

## Supporting Information

### A series of selective and sensitive fluorescent sensor based on thiophen-2-yl-benzothiazole unit for $\text{Hg}^{2+}$

Qunbo Mei,<sup>a\*</sup> Ruqiang Tian,<sup>a</sup> Yujie Shi,<sup>a</sup> Qingfang Hua,<sup>a</sup> Chen Chen,<sup>a</sup> Bihai Tong,<sup>b\*</sup>

<sup>a</sup> Key Laboratory for Organic Electronics & Information Displays (KLOEID), Institute of Advanced Materials (IAM), Nanjing University of Posts and Telecommunications (NUPT), Nanjing 210046, China;

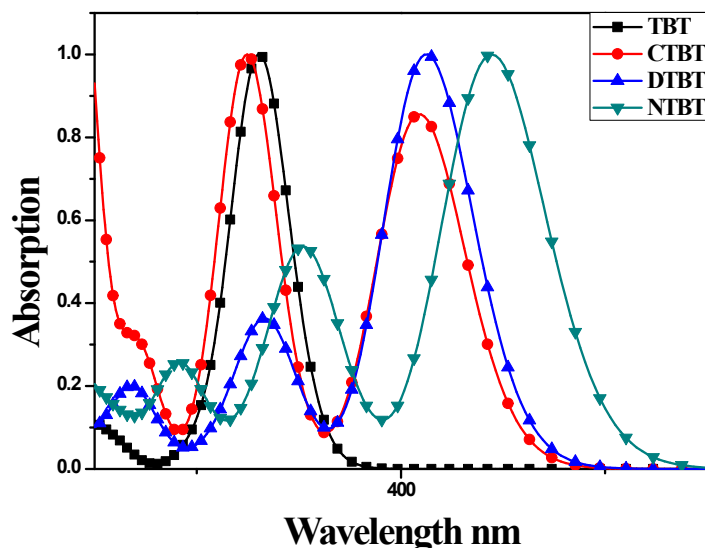
<sup>b</sup> Institute of Molecular Engineering and Applied Chemistry, College of Metallurgy and Resources, Anhui University of Technology, Ma'anshan, Anhui 243002, P. R. China.

#### Contents:

#### 1. Supplementary spectra data (Figure S1- Figure S8)

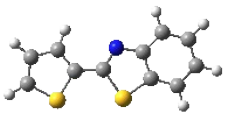
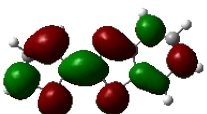
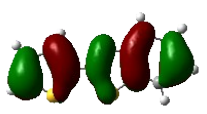
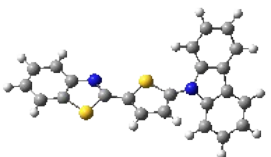
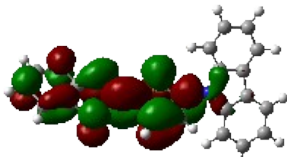
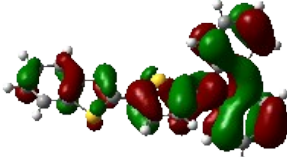
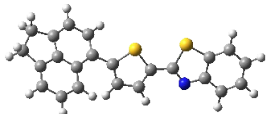
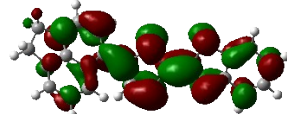

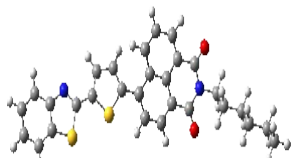
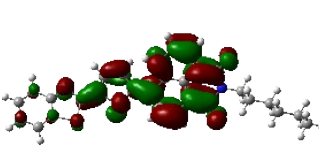
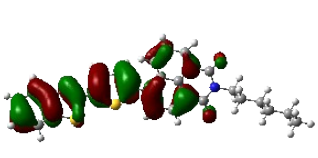
#### 2. Theoretical calculations data (Table S1- Table S5)

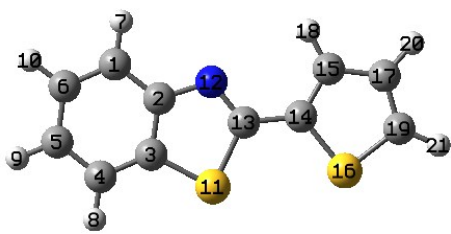
#### 3. GC-MS, MALDI-TOF mass, IR and NMR data (Figure S9- Figure S45)



**Figure S1.** UV-vis spectra of compounds TBT, CTBT, DTBT, and NTBT by density functional theory (DFT) in dichloromethane solution.

**Table S1.** The HOMO and LUMO distributions of TBT, CTBT, DTBT, and NTBT

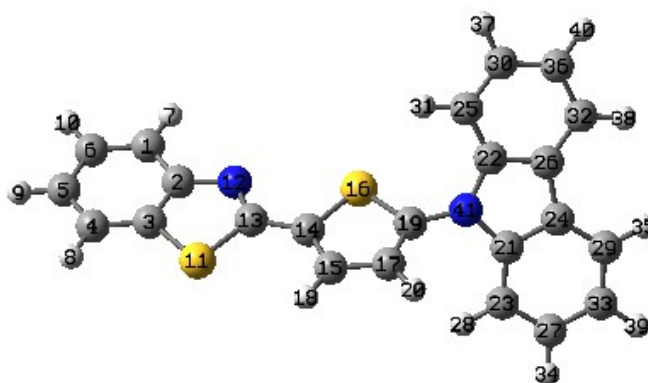
Molecular Structure	LUMO	HOMO
		
		
		
		

**Table S2.** The optimized geometry of TBT in ground state at B3LYP/6-31G(d)

Center number	Atom	Coordinates		
		X	Y	Z
1	C	-2.87587500	1.60385400	0.00015800
2	C	-1.76276900	0.74869800	0.00000500
3	C	-1.96408000	-0.65482800	-0.00007900
4	C	-3.24510700	-1.20923300	0.00002200
5	C	-4.33504100	-0.34157400	0.00009200
6	C	-4.15077400	1.05211300	0.00015200
7	H	-2.71858700	2.67776900	0.00014700
8	H	-3.39160900	-2.28506100	0.00006300
9	H	-5.34131300	-0.75083900	0.00014300
10	H	-5.01860800	1.70552400	0.00017900
11	S	-0.40749100	-1.45985000	-0.00028000

12	N	-0.44546800	1.16226400	-0.00007700
13	C	0.37268700	0.15082900	-0.00004100
14	C	1.81628100	0.29883300	-0.00013800
15	C	2.51116300	1.49003100	-0.00008100
16	S	2.91940800	-1.06077400	0.00029300
17	C	3.92054800	1.31429400	-0.00016200
18	H	2.00429300	2.44731700	-0.00024500
19	C	4.29170800	-0.00491600	0.00011700
20	H	4.63135200	2.13329400	-0.00041100
21	H	5.28961600	-0.42248100	0.00017600

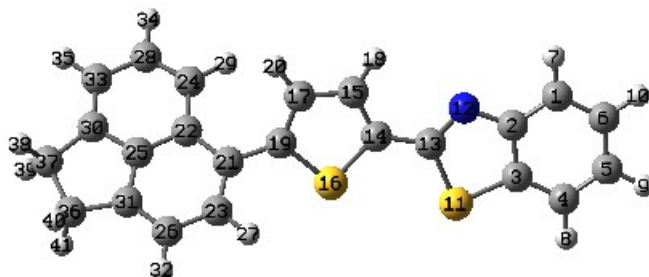
**Table S3.** The optimized geometry of CTBT in ground state at B3LYP/6-31G(d)



Center number	Atom	Coordinates		
		X	Y	Z
1	C	-5.39895900	1.40241100	-1.43628800
2	C	4.62202800	0.55418100	-0.63255900
3	C	-5.26324400	-0.38199100	0.21732500
4	C	-6.65415300	-0.48185100	0.27438300
5	C	-7.40617700	0.37021100	-0.53187100
6	C	-6.78351000	1.30329800	-1.37885800
7	H	-4.90354500	2.11726400	-2.08548600
8	H	-7.13990700	-1.20072500	0.92713300
9	H	-8.49042900	0.31011000	-0.50313300
10	H	-7.39467000	1.95510200	-1.99655000
11	S	-4.04929700	-1.29589600	1.09410900
12	N	-3.24148800	0.54426700	-0.59188700
13	C	-2.79366000	-0.34497500	0.24472700
14	C	-1.38860600	-0.57845300	0.49205200
15	C	-0.78788900	-1.47106800	1.35385100
16	S	-0.19898400	0.38288000	-0.35952100
17	C	0.62661700	-1.37825600	1.36667600
18	H	-1.34661000	-2.15876400	1.97986200
19	C	1.10525500	-0.41797600	0.50595500

20	H	1.27373800	-1.97919900	1.99487200
21	C	3.40724800	-1.04487600	-0.19875200
22	C	3.04961400	1.14550700	0.32360200
23	C	3.27053100	-2.40943600	-0.45546800
24	C	4.63622700	-0.36767100	-0.38658100
25	C	2.50305200	2.36408500	0.72909600
26	C	4.40890900	1.02514900	-0.05478700
27	C	4.39860100	-3.09931200	-0.89673400
28	H	2.31981100	-2.91482200	-0.32223400
29	C	5.75452600	-1.08407100	-0.82760900
30	C	3.34221800	3.47717500	0.73602600
31	H	1.46433000	2.44642900	1.03052200
32	C	5.23022800	2.15791000	-0.03772800
33	C	5.63006700	-2.44788400	-1.07825300
34	H	4.31972900	-4.16278100	-1.10497900
35	H	6.70600600	-0.58040700	-0.97617600
36	C	4.69085400	3.37970500	0.35532300
37	H	2.94111500	4.43838300	1.04515300
38	H	6.27565200	2.08311800	-0.32519000
39	H	6.49127900	-3.01461200	-1.42029000
40	H	5.31793900	4.26648900	0.37098000
41	N	2.44202100	-0.11972400	0.23916400

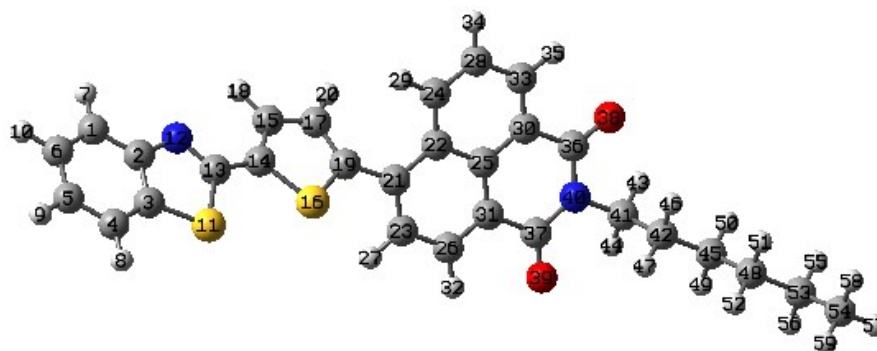
**Table S4.** The optimized geometry of **DTBT** in ground state at B3LYP/6-31G(d)



Center number	Atom	Coordinates		
		X	Y	Z
1	C	6.31924100	1.40212000	0.46634600
2	C	5.15830800	0.65483700	0.21193200
3	C	5.27380200	-0.62662600	-0.38469800
4	C	6.51574800	-1.16424900	-0.72621900
5	C	7.65415600	-0.40486800	-0.46460900
6	C	7.55529700	0.86674500	0.12651700
7	H	6.22794800	2.38262600	0.92283600
8	H	6.59627500	-2.14613000	-1.18271000
9	H	8.63119200	-0.80384300	-0.72221900
10	H	8.45908000	1.43777000	0.31961900

11	S	3.67535000	-1.31811800	-0.57841200
12	N	3.87233000	1.06666800	0.49712900
13	C	2.99507700	0.16841200	0.15244300
14	C	1.56890100	0.33778400	0.34116500
15	C	0.94993800	1.41990200	0.93309900
16	S	0.38375300	-0.83999700	-0.17611500
17	C	-0.45951200	1.30313900	0.97971600
18	H	1.51456100	2.25642700	1.32705700
19	C	-0.94312300	0.13167600	0.43015200
20	H	-1.10583300	2.03982800	1.44284000
21	C	-2.32590600	-0.35656000	0.33826400
22	C	-3.40876000	0.51177700	-0.04588900
23	C	-2.61315200	-1.68879500	0.63644000
24	C	-3.33375800	1.87131000	-0.45635000
25	C	-4.70332700	-0.06243100	-0.04896700
26	C	-3.92020900	-2.23281600	0.60342100
27	H	-1.79491600	-2.33657600	0.93916500
28	C	-4.48186000	2.56415700	-0.79877900
29	H	-2.37068100	2.36476000	-0.52366000
30	C	-5.87572300	0.64753000	-0.39457500
31	C	-4.97342900	-1.41138500	0.26951300
32	H	-4.06720500	-3.27991600	0.85549100
33	C	-5.77088900	1.96932600	-0.76470400
34	H	-4.39405100	3.60083200	-1.11403600
35	H	-6.64334300	2.55620200	-1.04113200
36	C	-6.46501900	-1.66333500	0.14937800
37	C	-7.07053200	-0.28343500	-0.28087500
38	H	-7.79372400	0.08304400	0.45780300
39	H	-7.61188800	-0.36131700	-1.23128200
40	H	-6.89157200	-2.01234500	1.09757300
41	H	-6.67940900	-2.44348800	-0.59116000

**Table S5.** The optimized geometry of **NTBT** in ground state at B3LYP/6-31G(d)



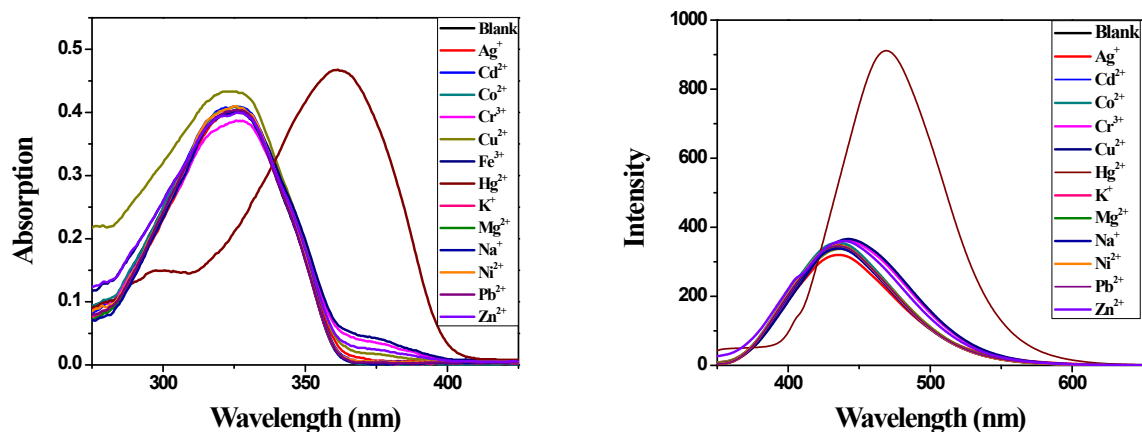
Center	Atom	Coordinates
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number		X	Y	Z
1	C	9.15789200	0.56046200	-0.17306000
2	C	7.87368000	-0.00714700	-0.17553300
3	C	7.72541200	-1.39285400	-0.43864800
4	C	8.82776100	-2.20930500	-0.69722500
5	C	10.09195600	-1.62453900	-0.68941400
6	C	10.25446800	-0.25217000	-0.42942600
7	H	9.26778600	1.62119800	0.02870300
8	H	8.70724800	-3.26936100	-0.89827900
9	H	10.96426000	-2.24081400	-0.88754400
10	H	11.25242900	0.17670700	-0.42972700
11	S	6.02582300	-1.81362000	-0.37214400
12	N	6.70233200	0.68275000	0.06185200
13	C	5.66572200	-0.10157000	-0.00314600
14	C	4.30942900	0.36518000	0.21237100
15	C	3.93682700	1.65251000	0.54222600
16	S	2.90688300	-0.66661000	0.06858100
17	C	2.53769700	1.81079200	0.67981700
18	H	4.66610400	2.44046300	0.68578700
19	C	1.82069000	0.65020500	0.46229400
20	H	2.06704700	2.74212400	0.97388800
21	C	0.37584700	0.40799700	0.58165400
22	C	-0.59335000	1.30957500	0.01435600
23	C	-0.07262500	-0.71501800	1.27243700
24	C	-0.25209800	2.42528900	-0.79567600
25	C	-1.98321900	1.05237200	0.24385900
26	C	-1.43939400	-0.96789000	1.46624300
27	H	0.65549700	-1.39253600	1.70773200
28	C	-1.22354800	3.26354500	-1.30607900
29	H	0.78976200	2.60606000	-1.03278600
30	C	-2.96257300	1.93398200	-0.28302100
31	C	-2.38949100	-0.09043700	0.97741900
32	H	-1.77088600	-1.83978600	2.02014800
33	C	-2.58535500	3.02803200	-1.04015200
34	H	-0.93562800	4.10635700	-1.92754000
35	H	-3.35858100	3.68052800	-1.43168200
36	C	-4.40837000	1.69140200	-0.04129600
37	C	-3.82623800	-0.36725100	1.22394600
38	O	-5.27853600	2.43248800	-0.48016900
39	O	-4.20700400	-1.35626200	1.83742500
40	N	-4.74568300	0.56594100	0.72410200
41	C	-6.17776900	0.31600000	0.97614300
42	C	-6.83248800	-0.52832600	-0.12241700
43	H	-6.65974100	1.29235600	1.04614900

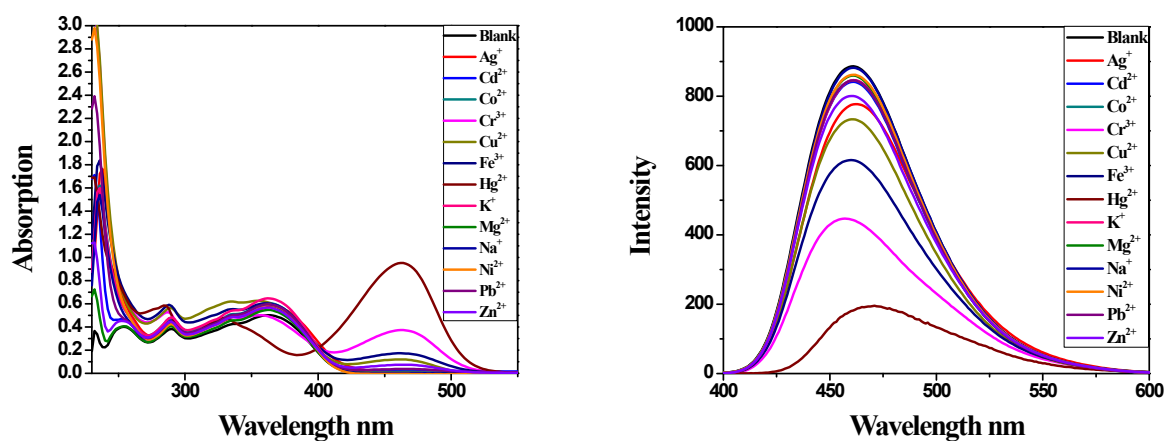
44	H	-6.24260400	-0.19304100	1.93896400
45	C	-8.31642100	-0.79128500	0.16296500
46	H	-6.72494800	-0.00717100	-1.08198200
47	H	-6.29574700	-1.48191200	-0.20433900
48	C	-9.00400400	-1.62039000	-0.92941600
50	H	-8.41524200	-1.30931300	1.12828200
51	H	-8.84254800	0.16832300	0.27436500
52	H	-8.91192800	-1.09807600	-1.89321700
53	H	-8.47214400	-2.57589500	-1.04937200
54	C	-10.48543900	-1.89894500	-0.64452400
55	C	-11.16757700	-2.72051500	-1.74315100
56	H	-11.01576600	-0.94420300	-0.51886200
57	H	-10.57598300	-2.42547900	0.31624300
58	H	-12.22208900	-2.90572500	-1.50858500
59	H	-11.12742300	-2.20164800	-2.70890300
60	H	-10.67893400	-3.69432600	-1.87142400

**Table S6.** The frontier molecular orbital energies of **TBT**, **CTBT**, **DTBT**, and **NTBT**.

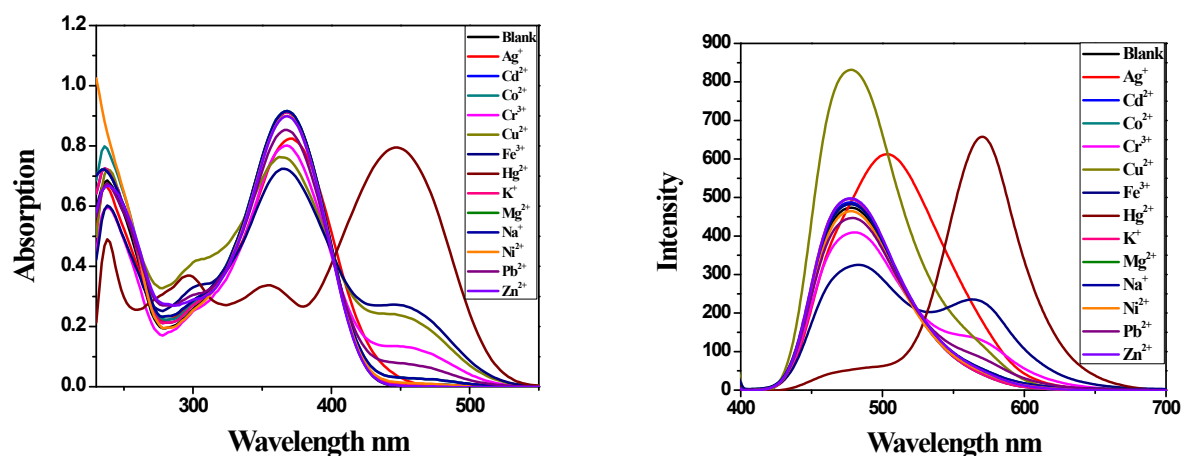
Molecular	LUMO	HOMO
<b>TBT</b>	-1.73 eV	-5.86 eV
<b>CTBT</b>	-1.90 eV	-5.45 eV
<b>DTBT</b>	-1.82 eV	-5.33 eV
<b>NTBT</b>	-2.66 eV	-5.90 eV



**Figure S2.** UV-vis spectra and emission spectra of **TBT** ( $c = 2.0 \times 10^{-5}$  M) in the presence of metal ions in dichloromethane.  $\text{Ag}^+$ ,  $\text{Cd}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Hg}^{2+}$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Na}^+$ ,  $\text{Ni}^{2+}$ ,  $\text{Pb}^{2+}$  and  $\text{Zn}^{2+}$  (2.0 equiv) were added, respectively.

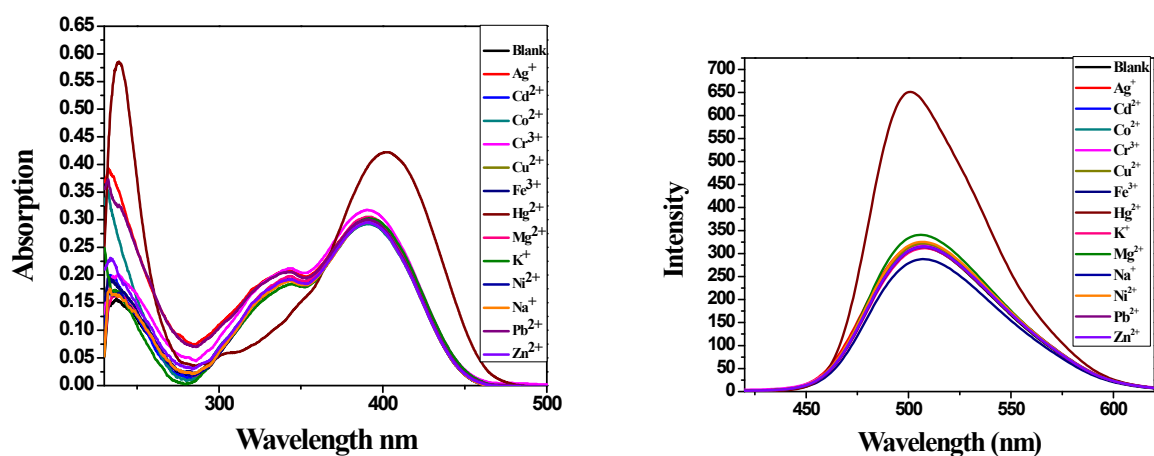


**Figure S3.** UV-vis spectra and emission spectra of **CTBT** ( $c = 2.0 \times 10^{-5}$  M) in the presence of metal ions in dichloromethane.  $\text{Ag}^+$ ,  $\text{Cd}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Hg}^{2+}$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Na}^+$ ,  $\text{Ni}^{2+}$ ,  $\text{Pb}^{2+}$  and  $\text{Zn}^{2+}$  (2.0 equiv) were added, respectively.

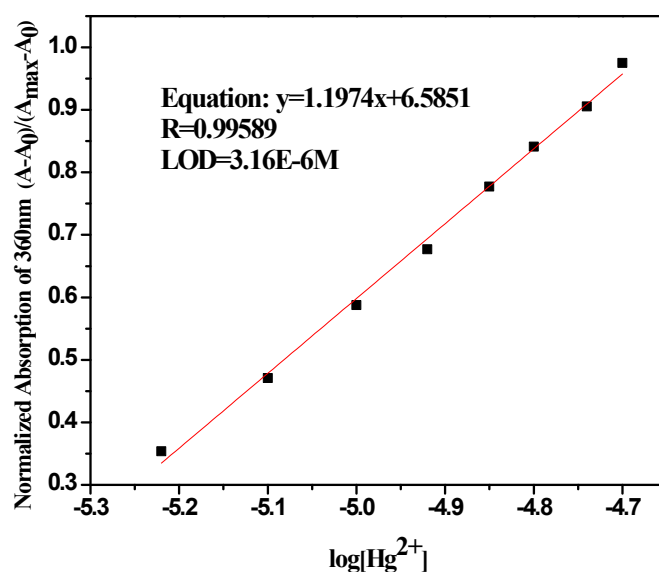


**Figure S4.** UV-vis spectra and emission spectra of **DTBT** ( $c = 2.0 \times 10^{-5}$  M) in the presence of metal ions in dichloromethane.  $\text{Ag}^+$ ,  $\text{Cd}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Hg}^{2+}$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Na}^+$ ,  $\text{Ni}^{2+}$ ,  $\text{Pb}^{2+}$  and  $\text{Zn}^{2+}$  (2.0 equiv) were added, respectively.

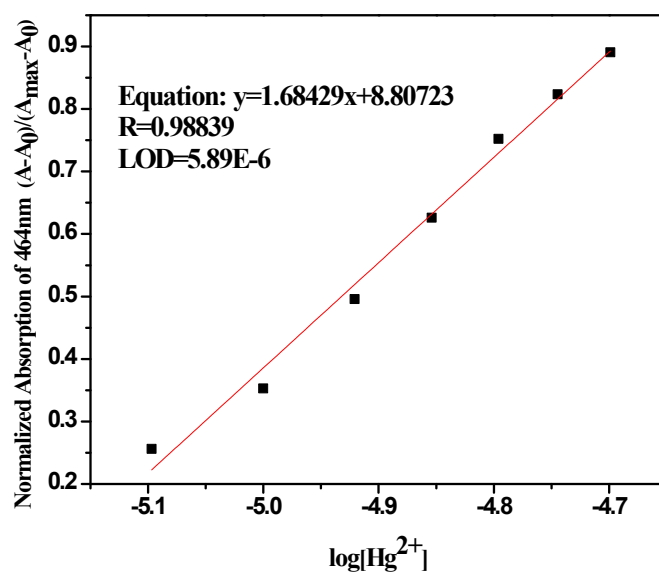




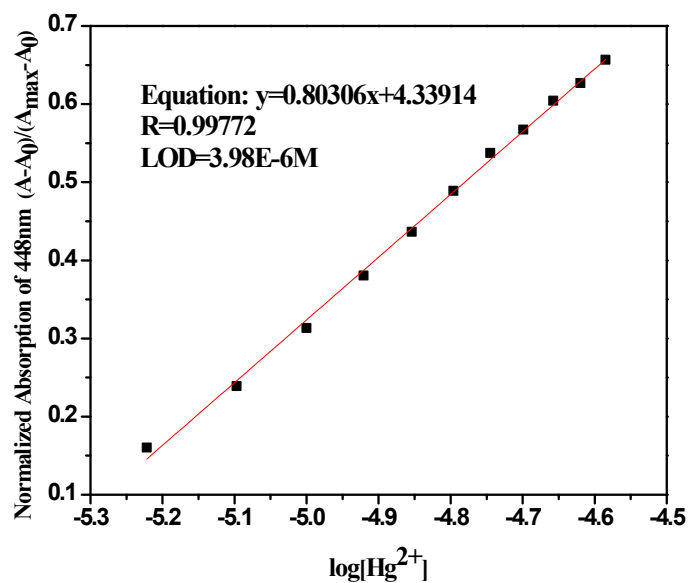
**Figure S5.** UV-vis spectra and emission spectra of NTBT ( $c = 2.0 \times 10^{-5}$  M) in the presence of metal ions in dichloromethane.  $\text{Ag}^+$ ,  $\text{Cd}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Hg}^{2+}$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Na}^+$ ,  $\text{Ni}^{2+}$ ,  $\text{Pb}^{2+}$  and  $\text{Zn}^{2+}$  (2.0 equiv) were added, respectively.



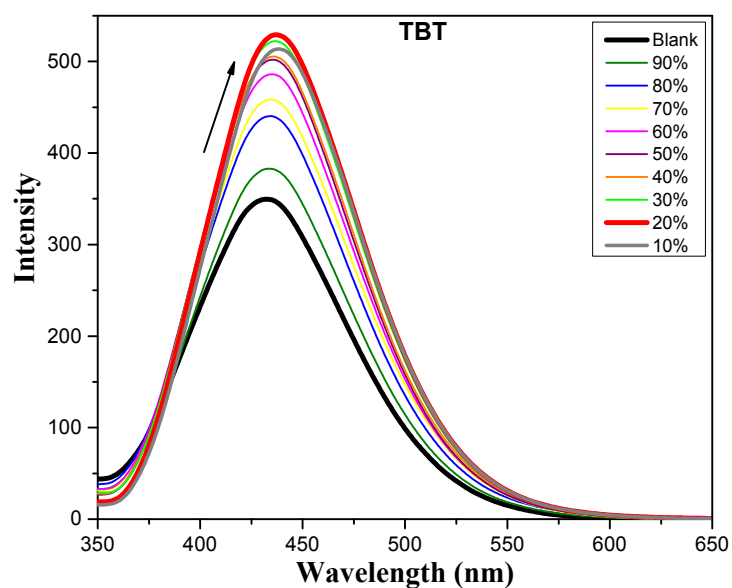
**Figure S6.** Absorption intensity of the TBT at various concentration of  $\text{Hg}^{2+}$ . (The fitted line of the eight intermediate values (6  $\mu\text{M}$  -20  $\mu\text{M}$   $\text{Hg}^{2+}$ ).



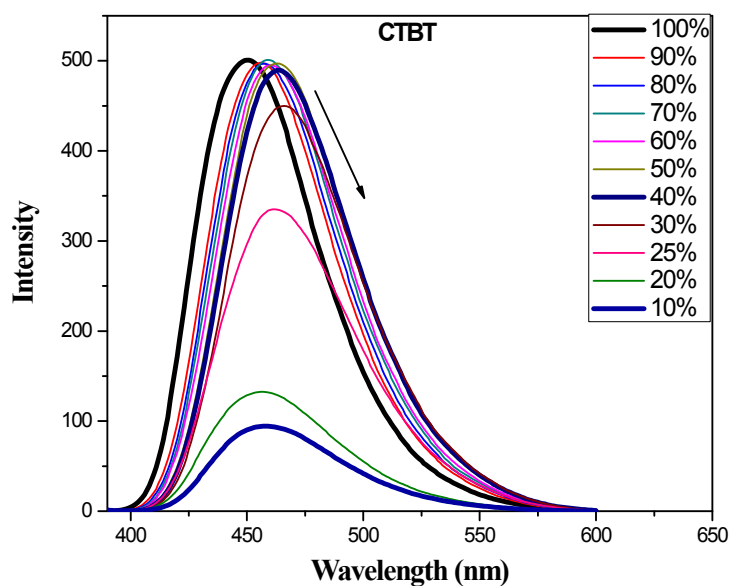
**Figure S7.** Absorption intensity of the CTBT at various concentration of  $\text{Hg}^{2+}$ . (The fitted line of the seven intermediate values (8  $\mu\text{M}$  -20  $\mu\text{M}$   $\text{Hg}^{2+}$ ).



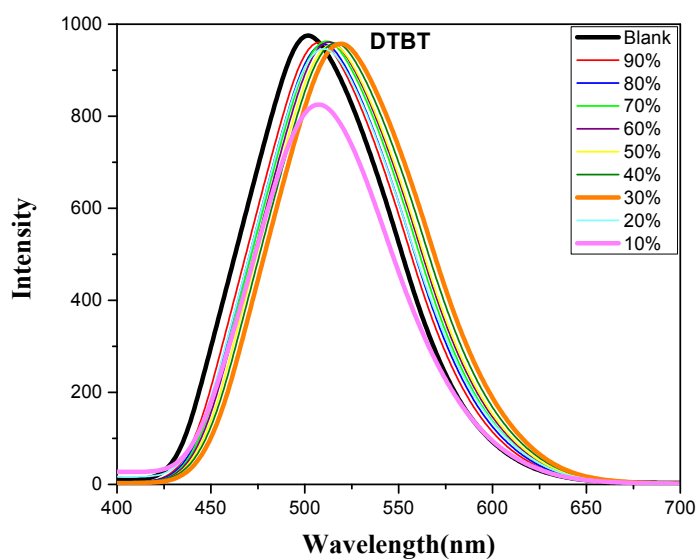
**Figure S8.** Absorption intensity of the DTBT at various concentration of  $\text{Hg}^{2+}$ . (The fitted line of the eleven intermediate values (6  $\mu\text{M}$  -26  $\mu\text{M}$   $\text{Hg}^{2+}$ ).



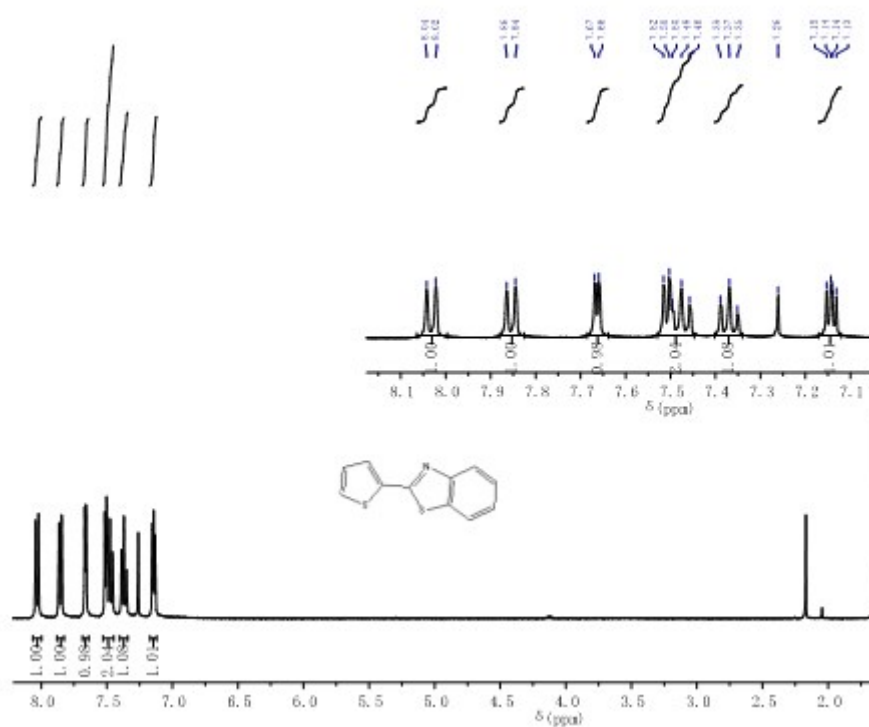
**Figure S9.** Changes in the luminescent spectra of **TBT** ( $c=2\times 10^{-5}$  M) in THF and the mixed solvent of THF and water (different volume ratio).



**Figure S10.** Changes in the luminescent spectra of **CTBT** ( $c=2\times 10^{-5}$  M) in THF and the mixed solvent of THF and water (different volume ratio).



**Figure S11.** Changes in the luminescent spectra of **DTBT** ( $c=2 \times 10^{-5}$  M) in THF and the mixed solvent of THF and water (different volume ratio).



**Figure S12.**  $^1\text{H}$  NMR spectrum of **TBT**

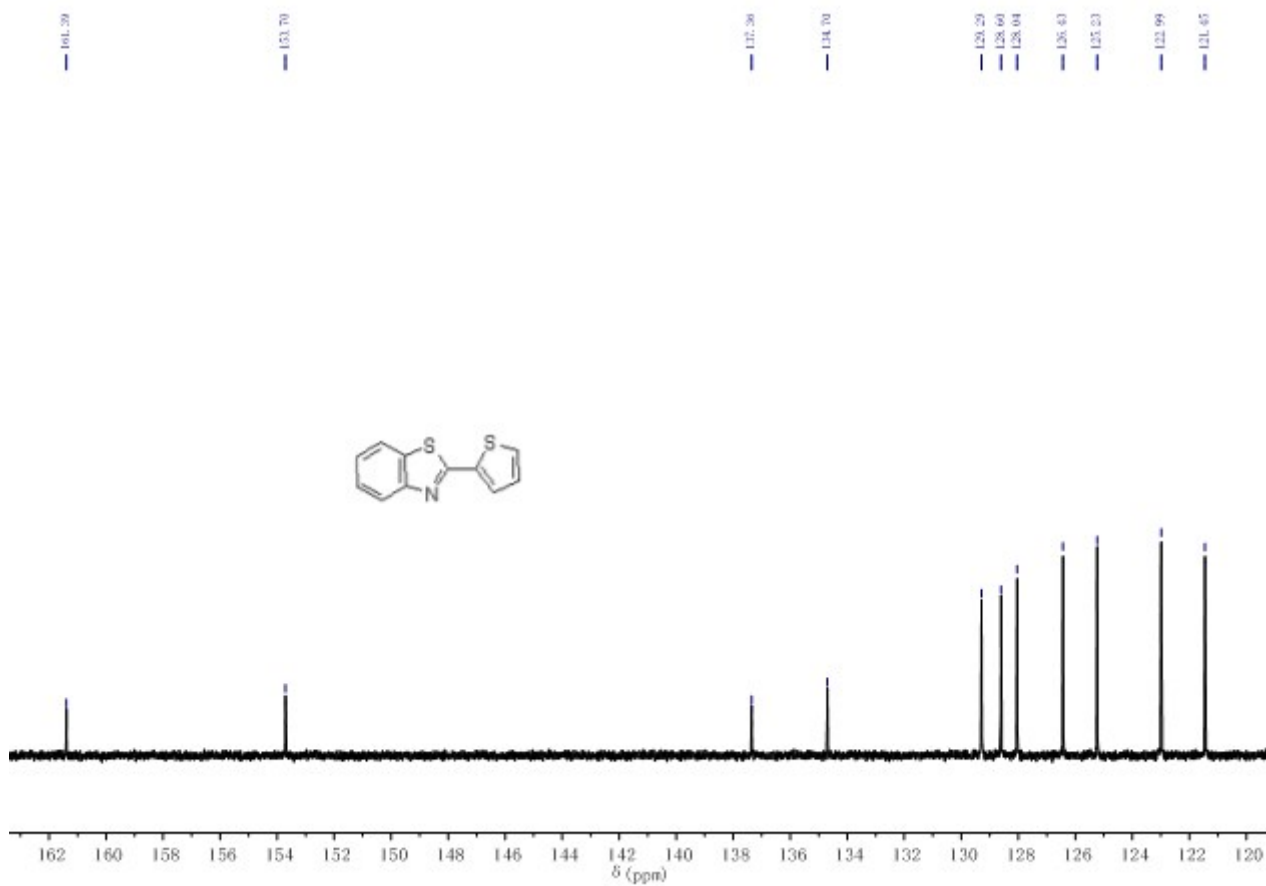


Figure S13.  $^{13}\text{C}$  NMR spectrum of TBT

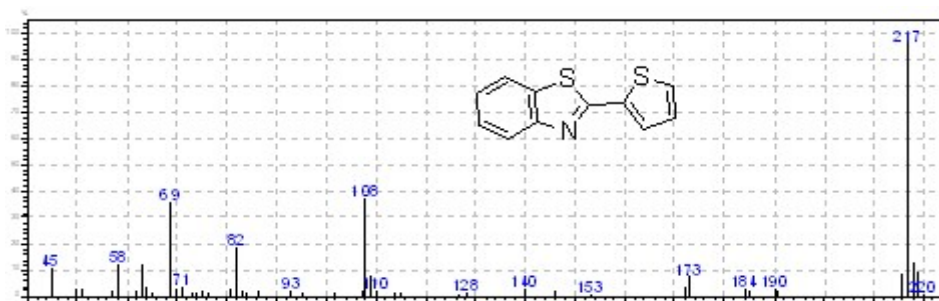


Figure S14. GC-MS of TBT

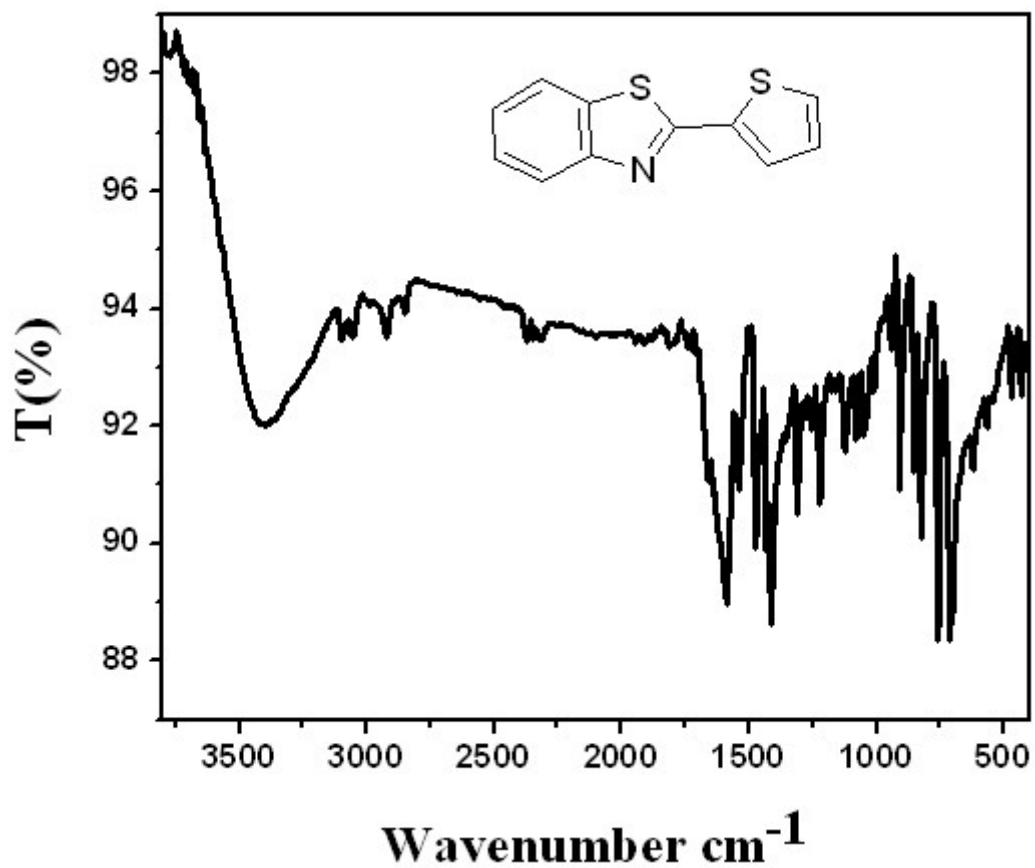


Figure S15. IR spectrum of TBT

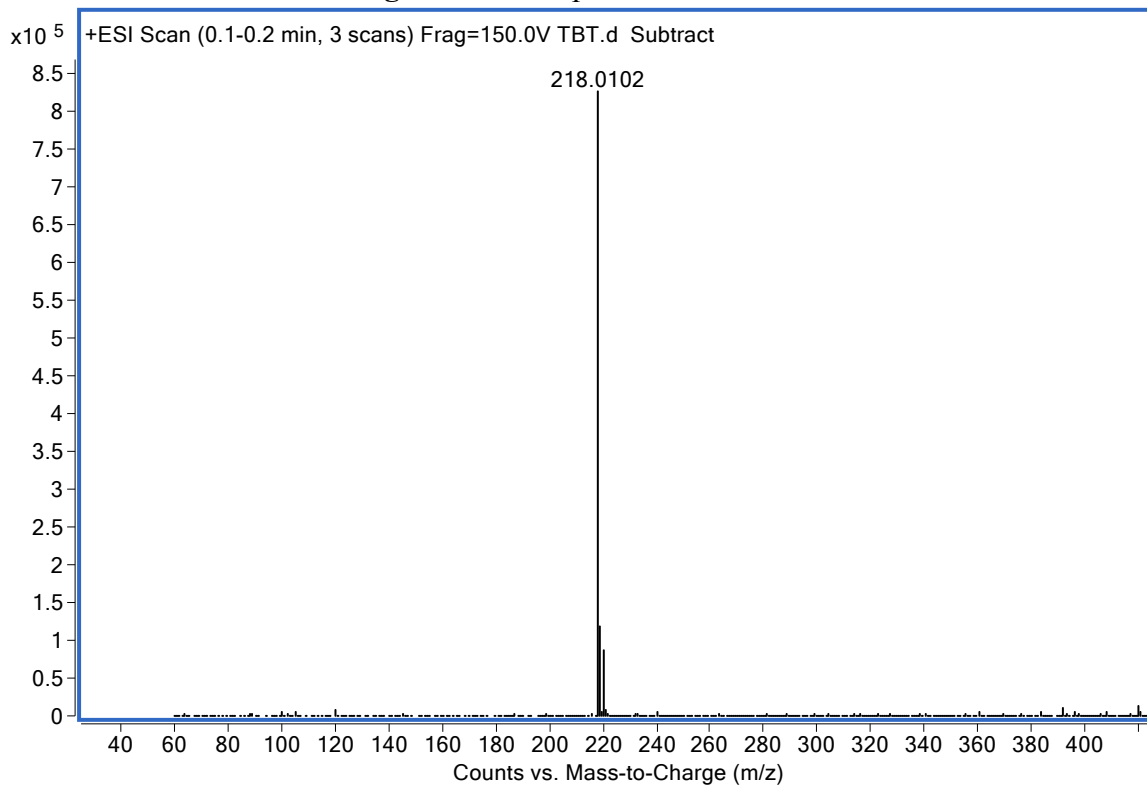
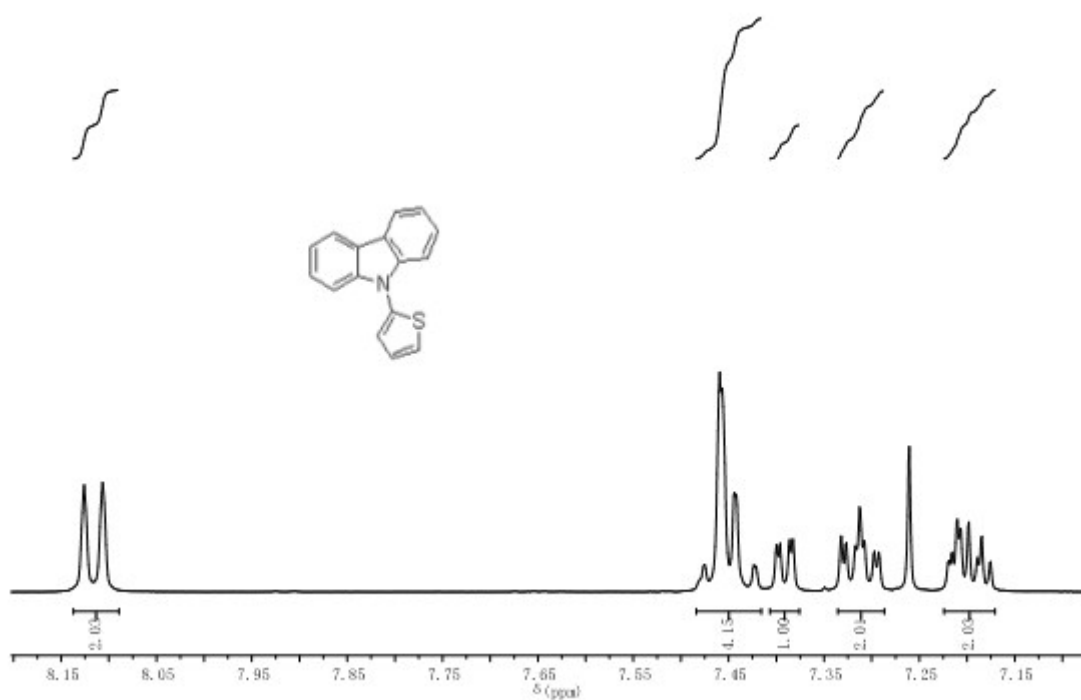
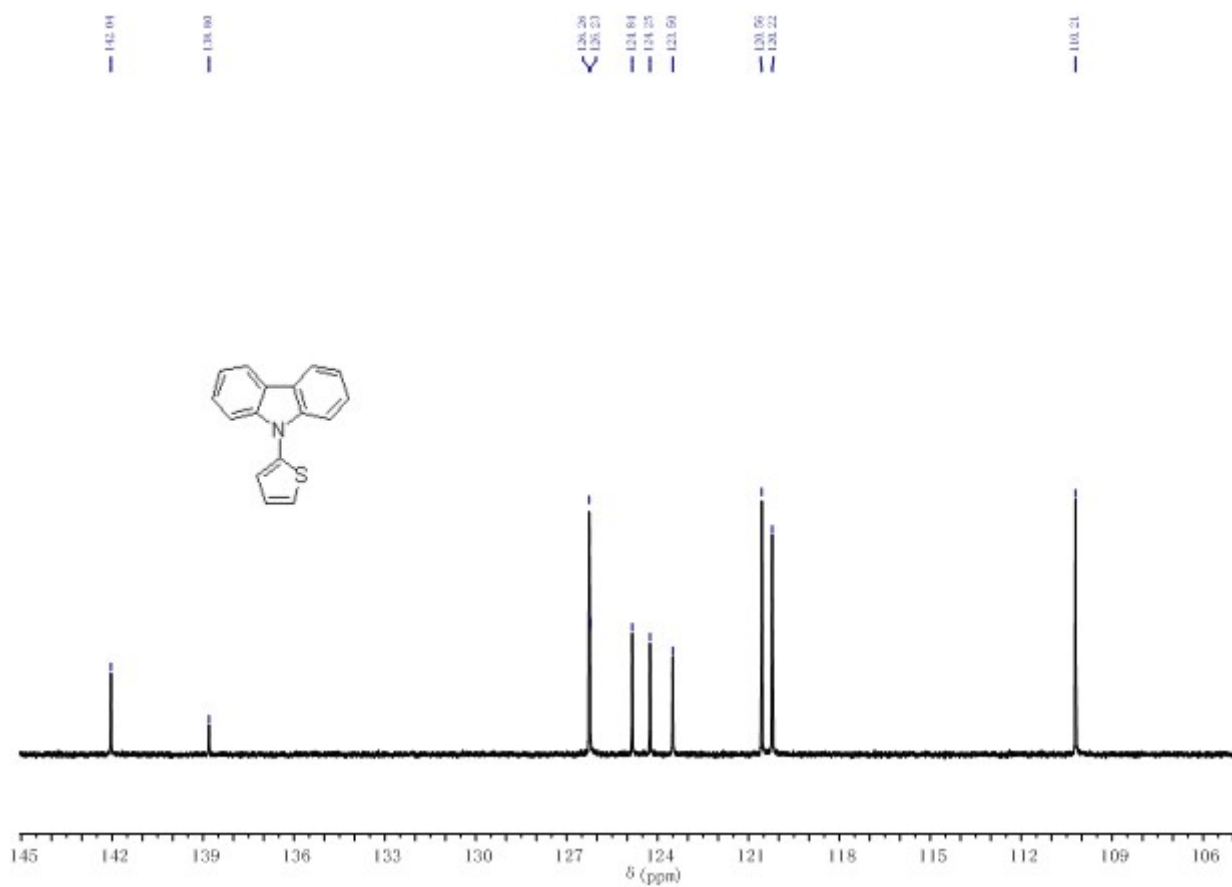


Figure S16. GC-MS of TBT



**Figure S17.**  $^1\text{H}$  NMR spectrum of 9-thiophen-2-yl-9H-Carbazole



**Figure S18.**  $^{13}\text{C}$  NMR spectrum of 9-thiophen-2-yl-9H-Carbazole

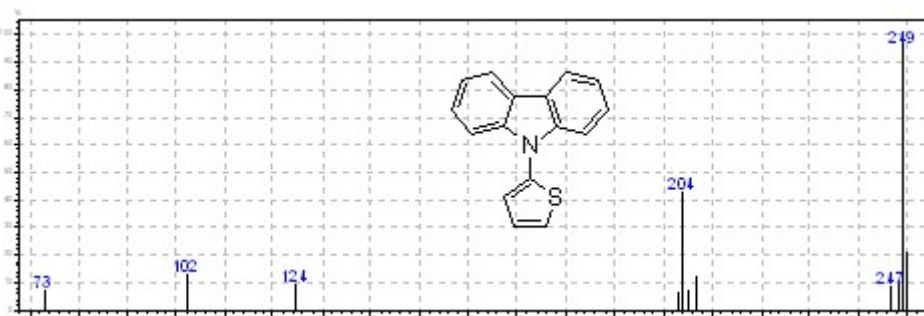


Figure S19. GC-MS of 9-thiophen-2-yl-9H-Carbazole

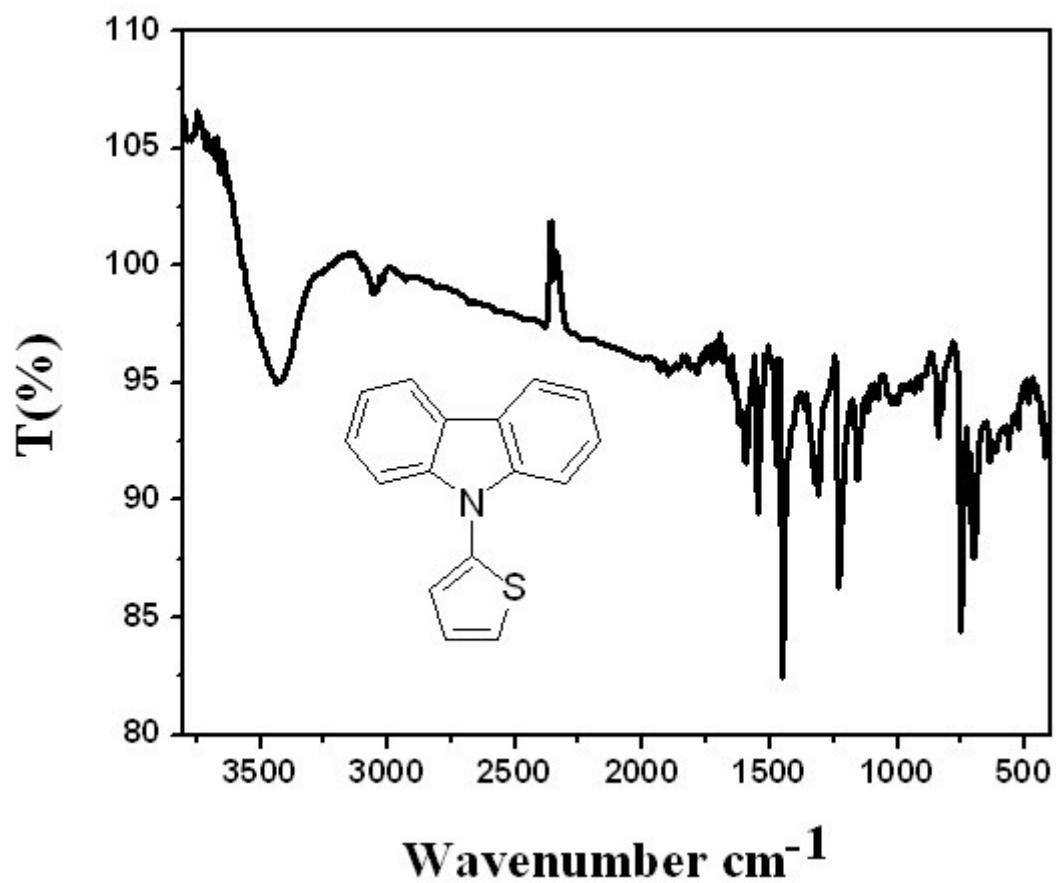
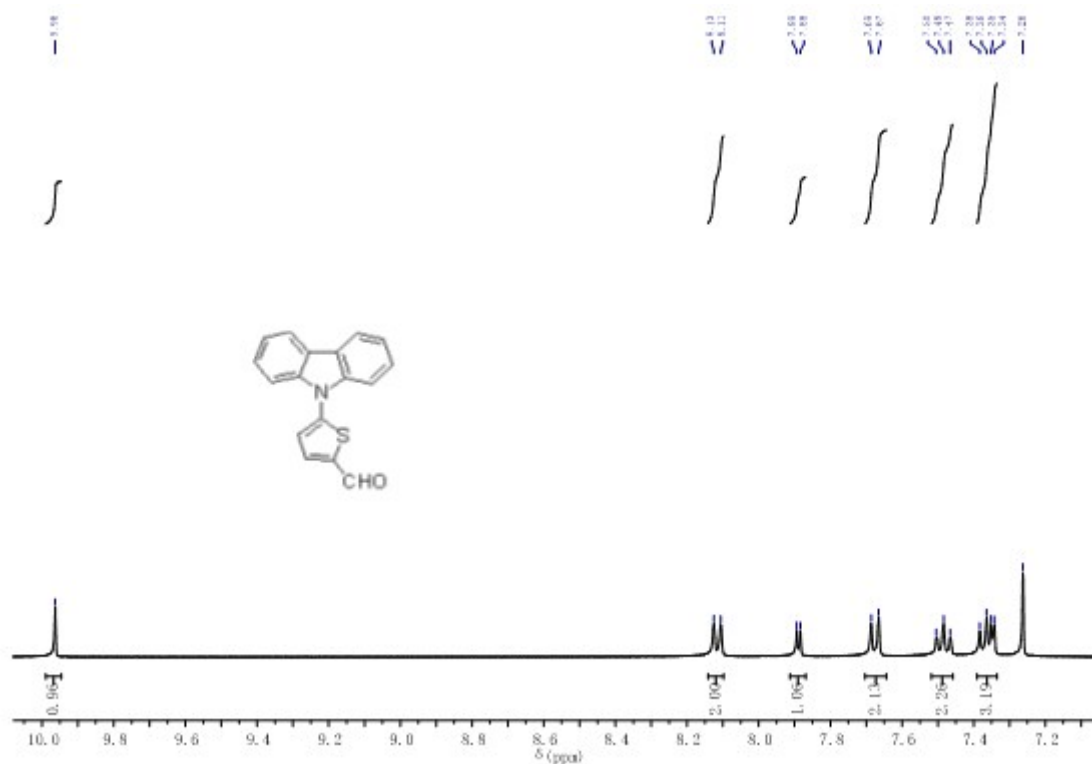
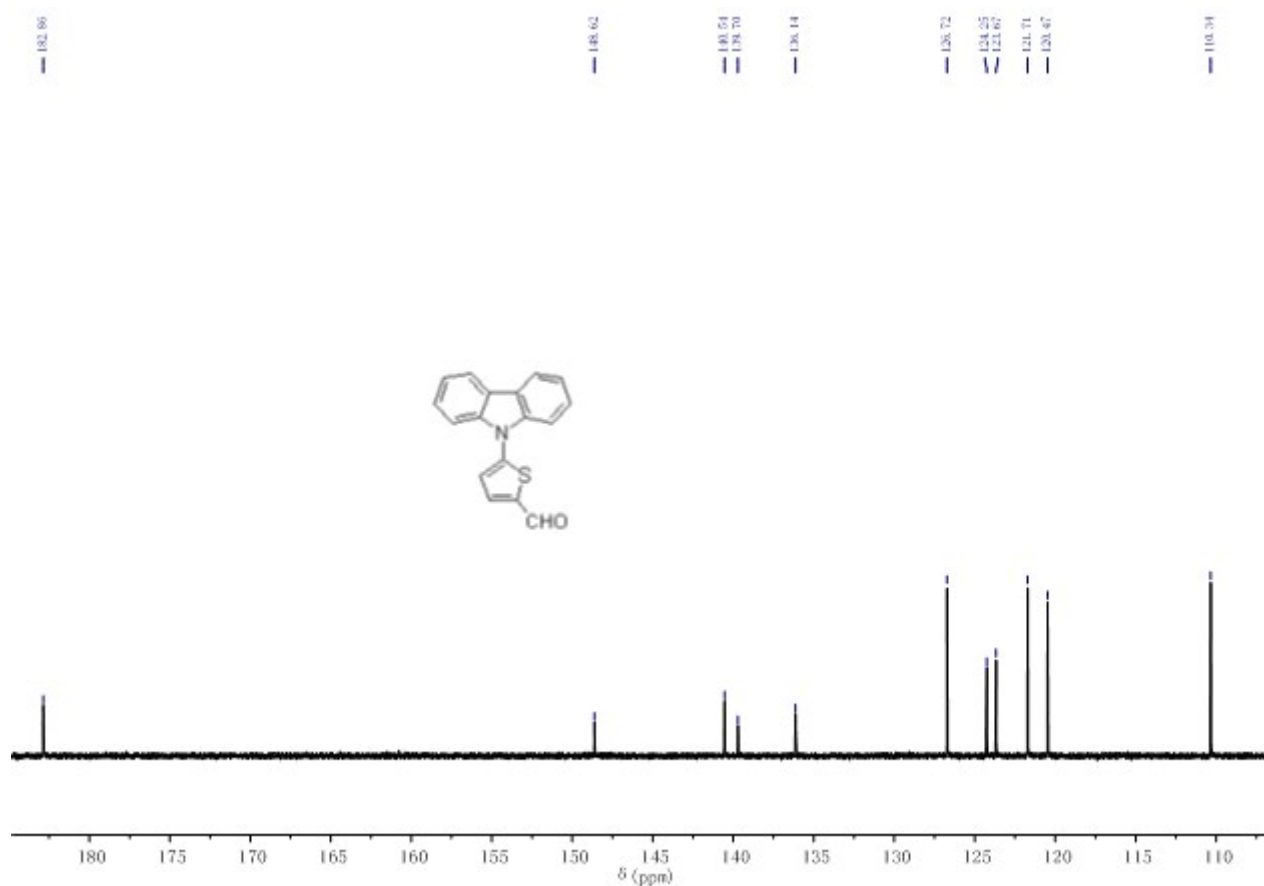


Figure S20. IR spectrum of 9-thiophen-2-yl-9H-Carbazole





**Figure S21.** <sup>1</sup>H NMR spectrum of 5-Carbazol-9-yl-thiophene-carbaldehyde



**Figure S22.** <sup>13</sup>C NMR spectrum of 5-Carbazol-9-yl-thiophene-carbaldehyde

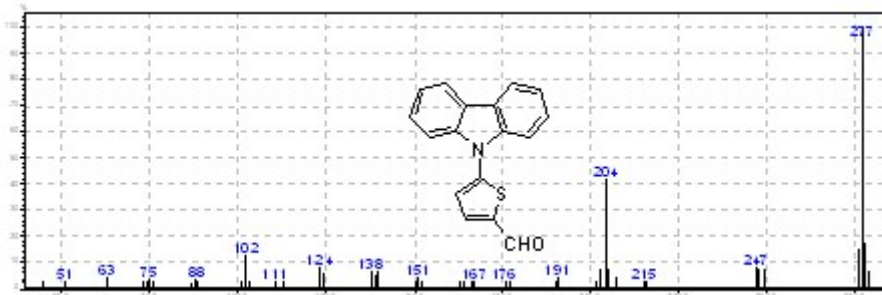


Figure S23. GC-MS of 5-Carbazol-9-yl-thiophene-carbaldehyde

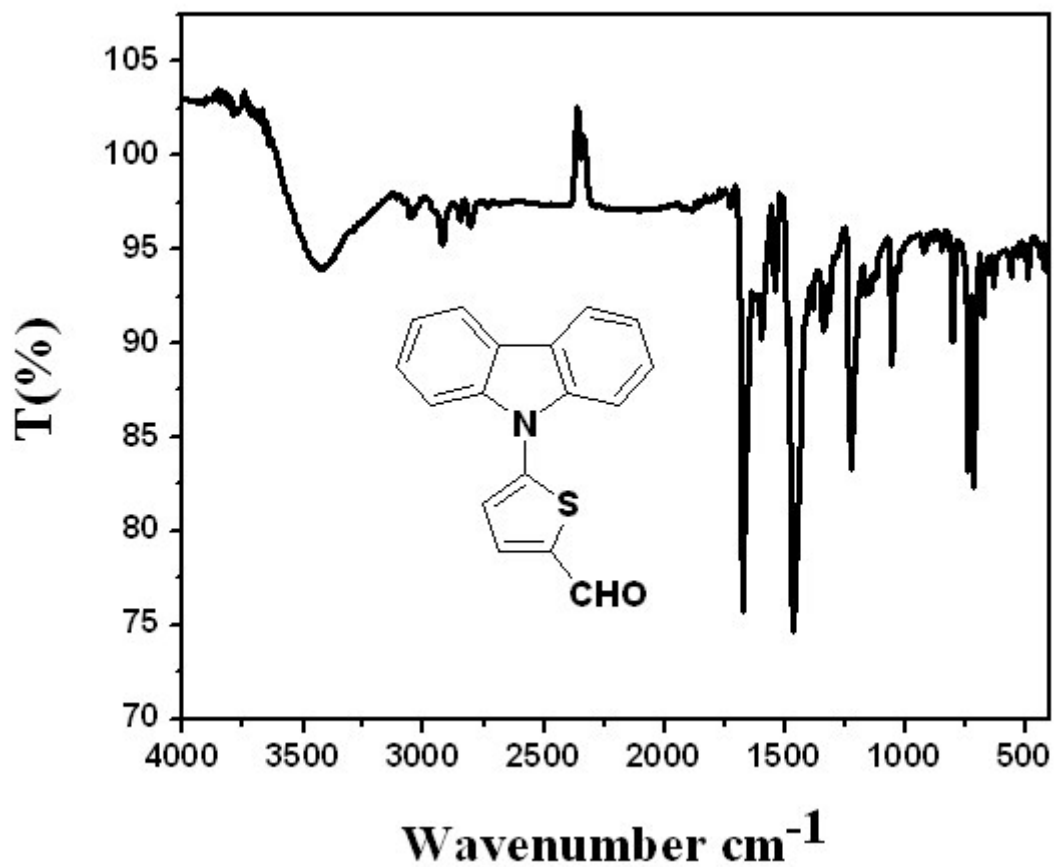


Figure S24. IR spectrum of 5-Carbazol-9-yl-thiophene-carbaldehyde

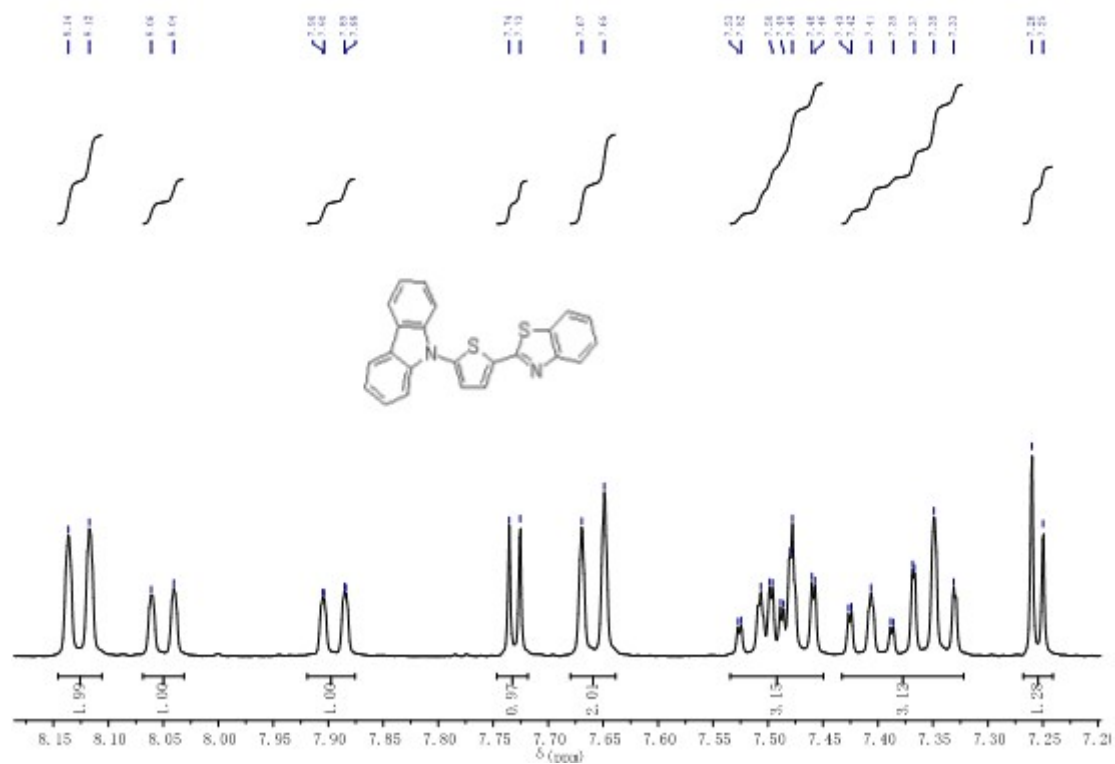


Figure S25.  $^1\text{H}$  NMR spectrum of CTBT

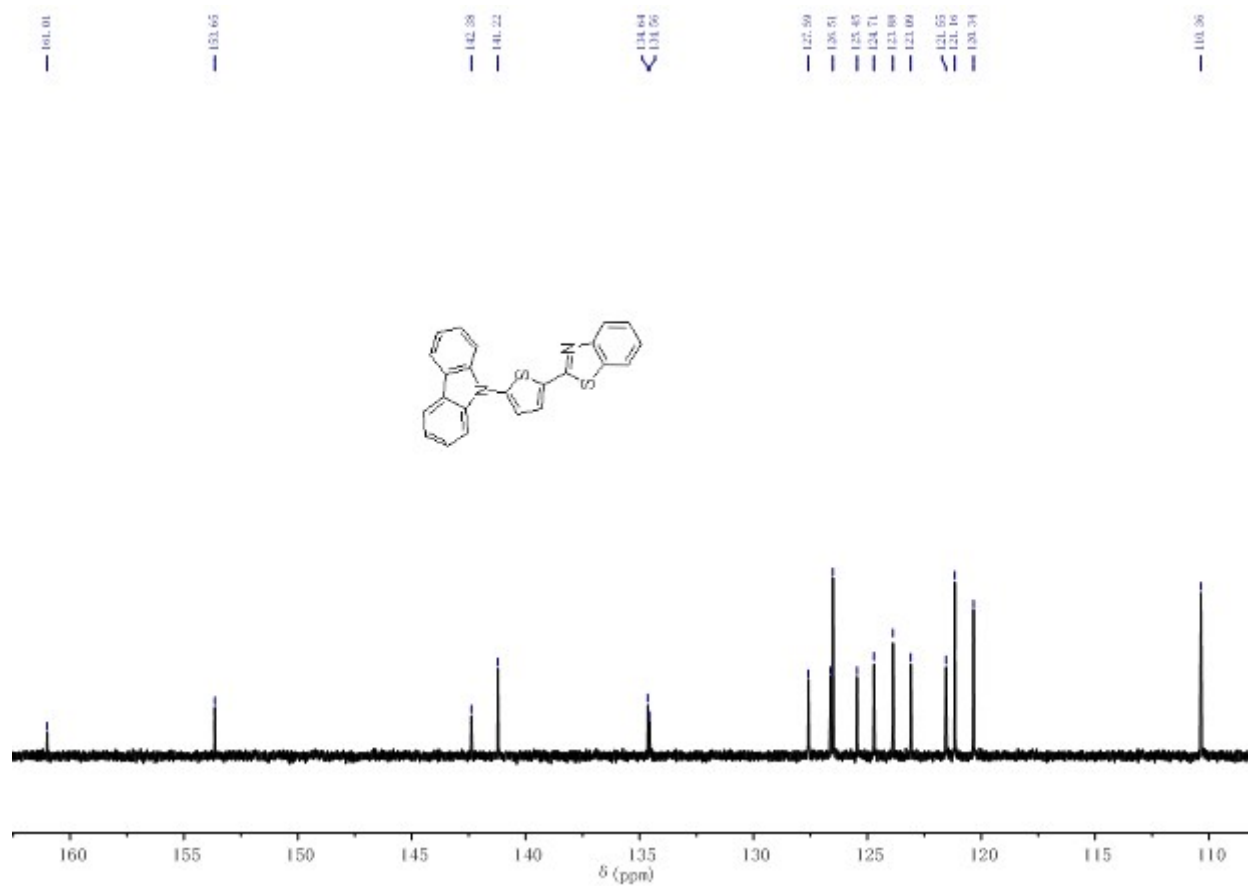


Figure S26.  $^{13}\text{C}$  NMR spectrum of CTBT

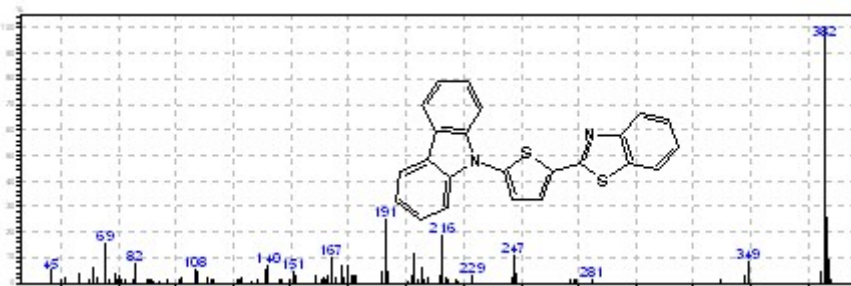


Figure S27. GC-MS of CTBT

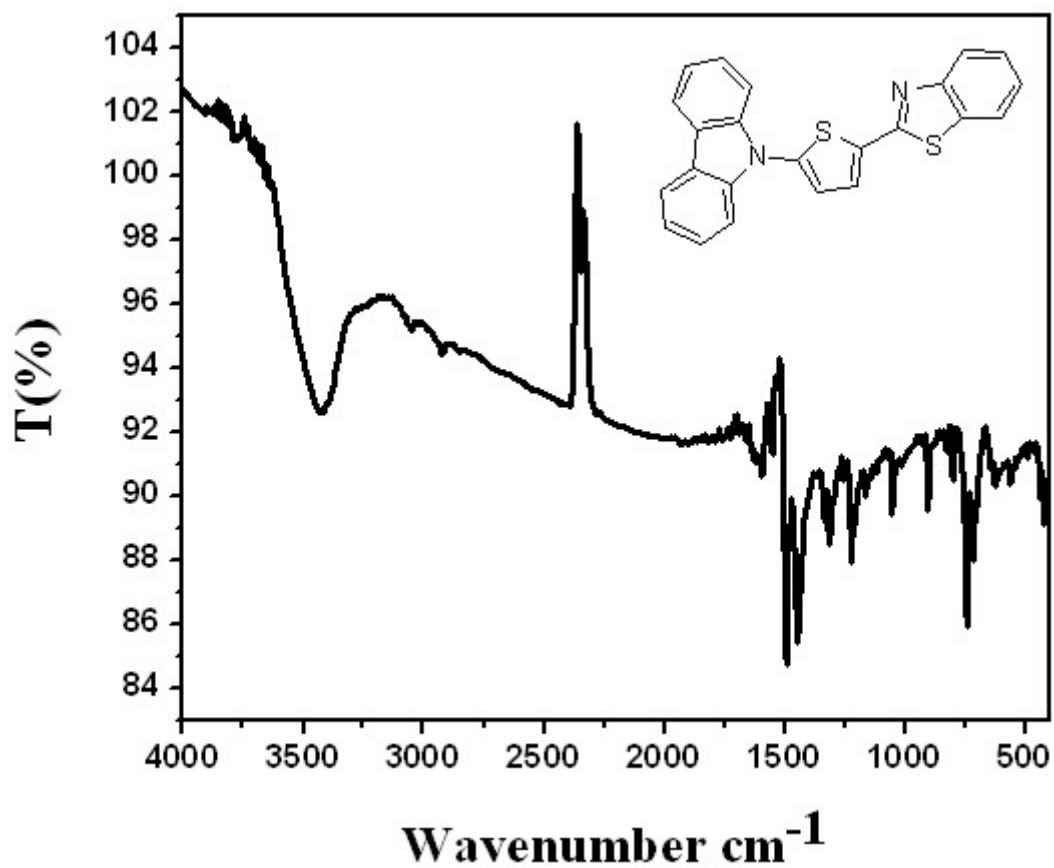
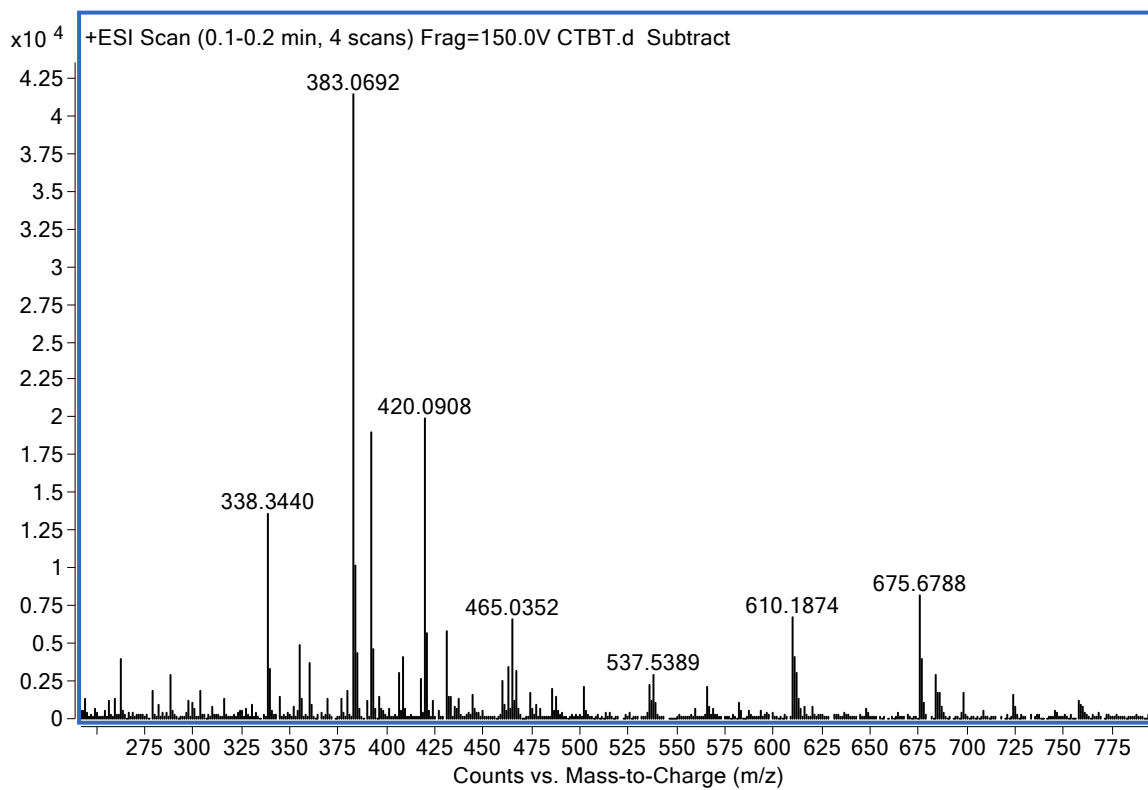
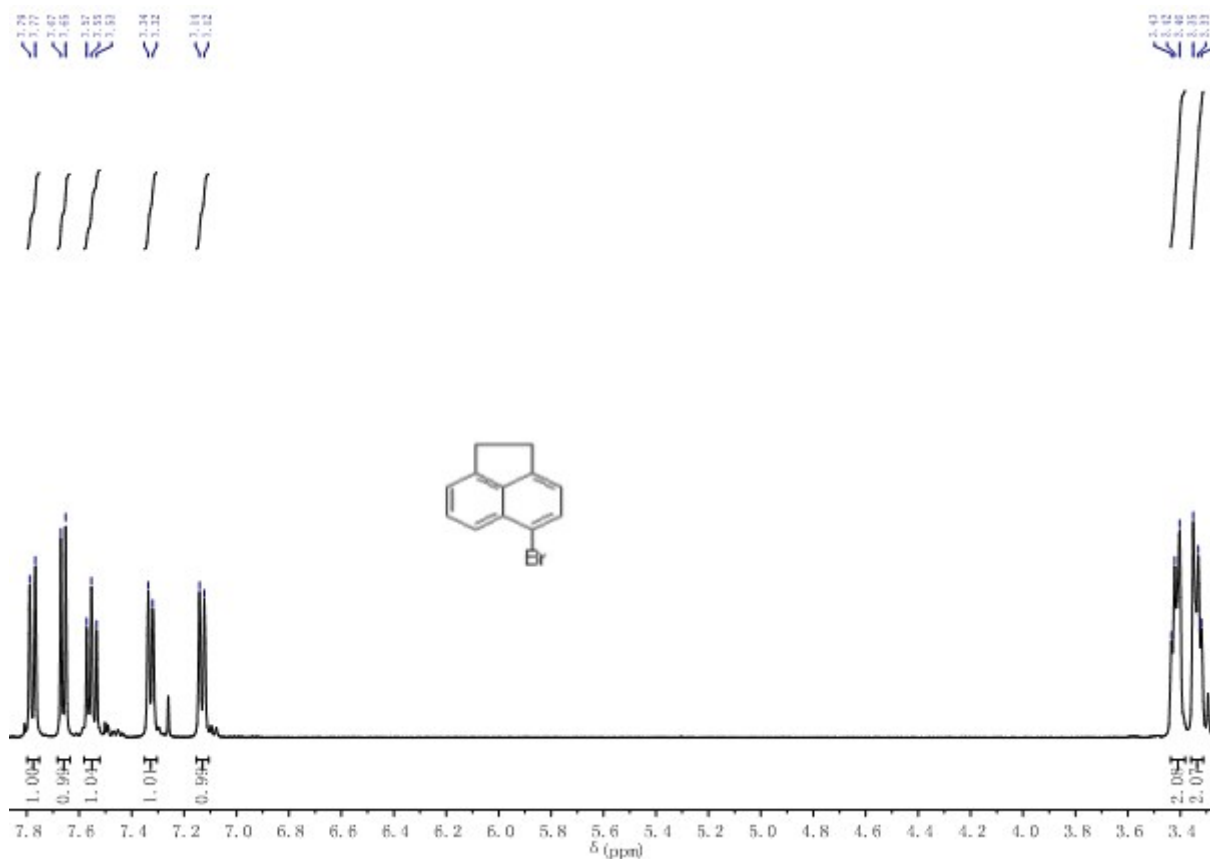


Figure S28. IR spectrum of CTBT



**Figure S29.** GC-MS of CTBT



**Figure S30.** <sup>1</sup>H NMR spectrum of 5-bromo-acenaphthene

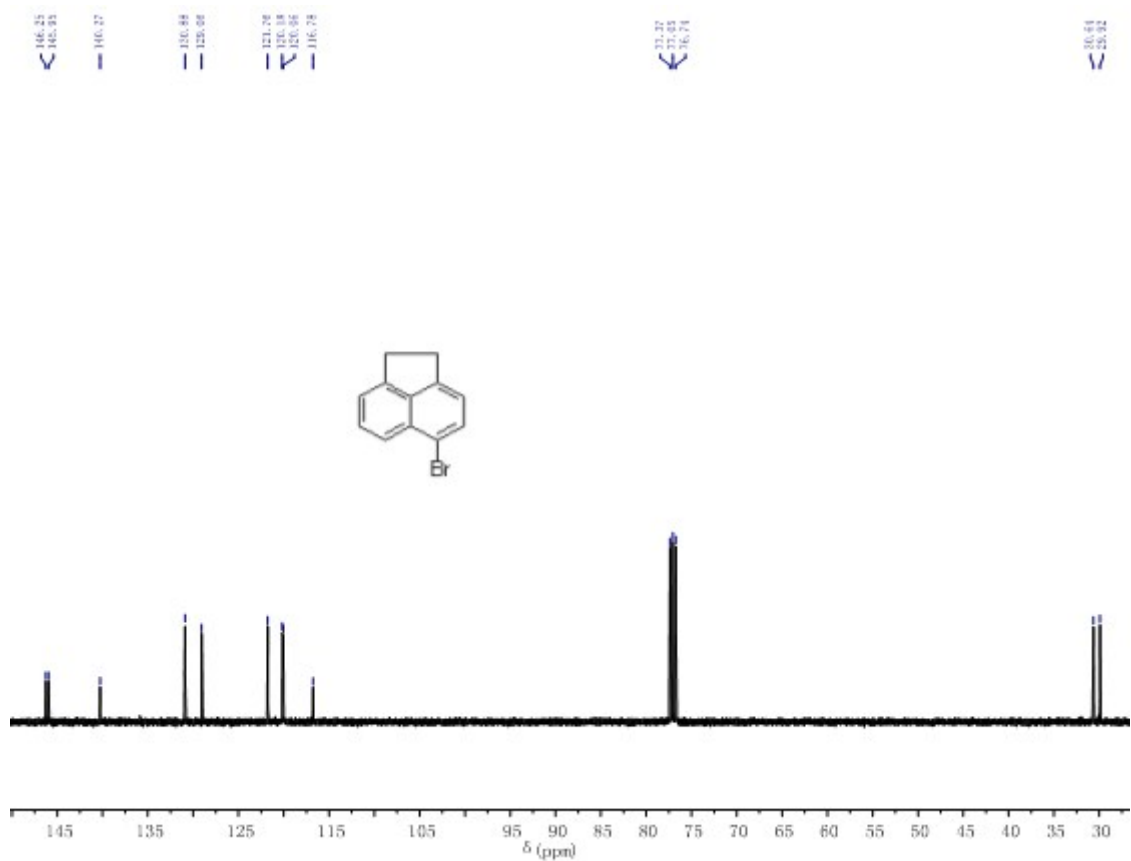


Figure S31.  $^{13}\text{C}$  NMR spectrum of 5-bromo-acenaphthene

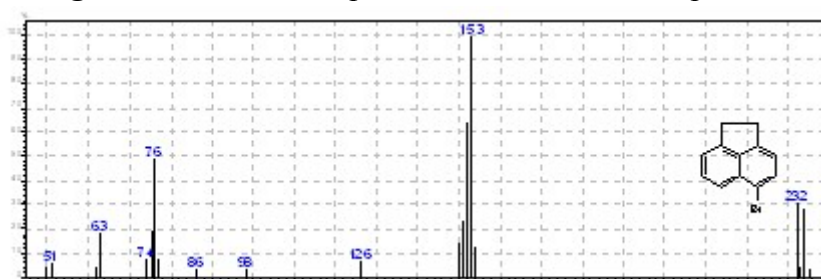
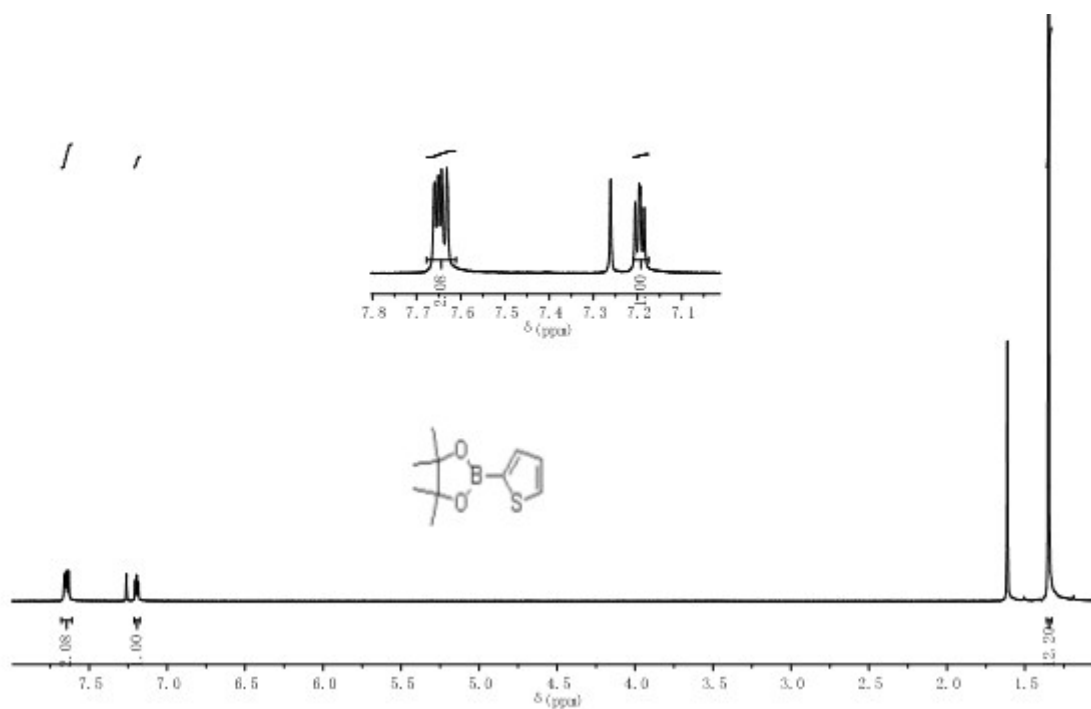
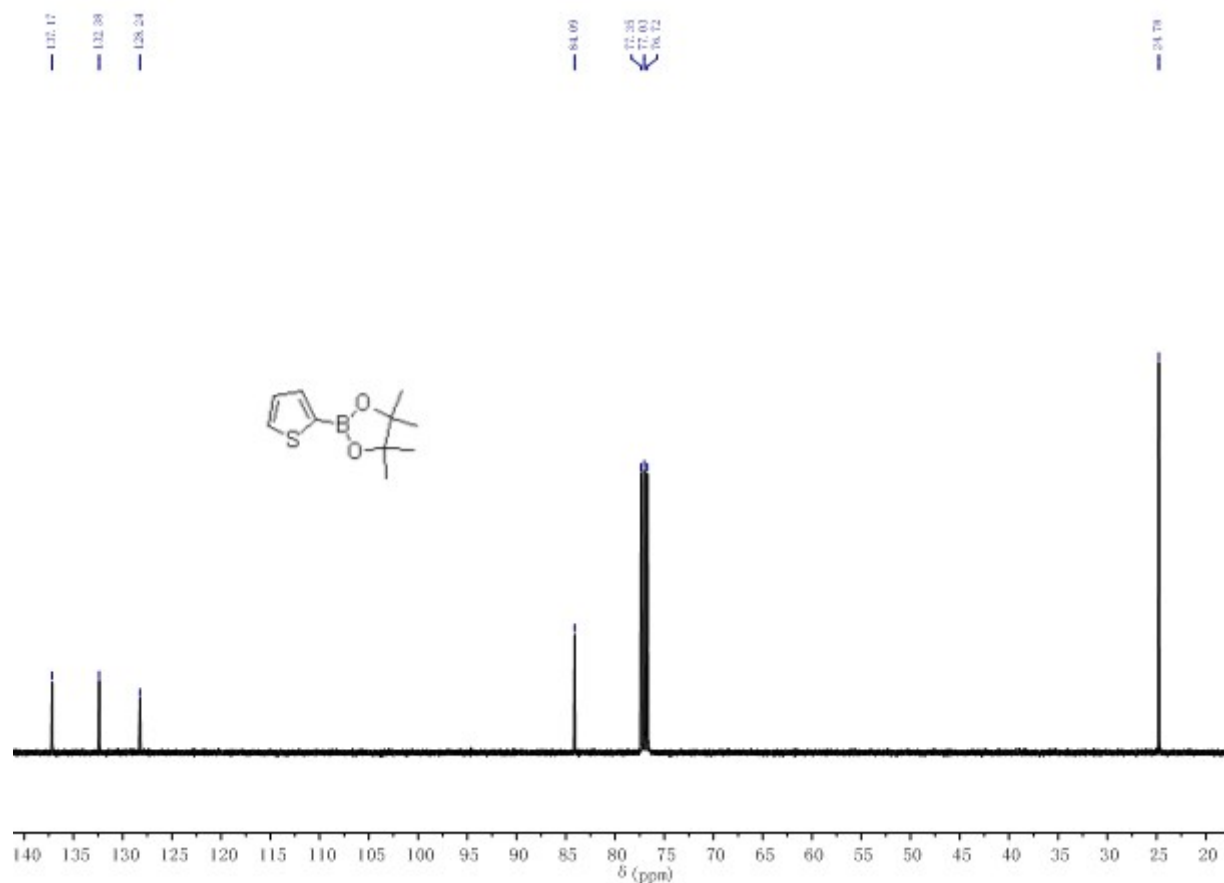


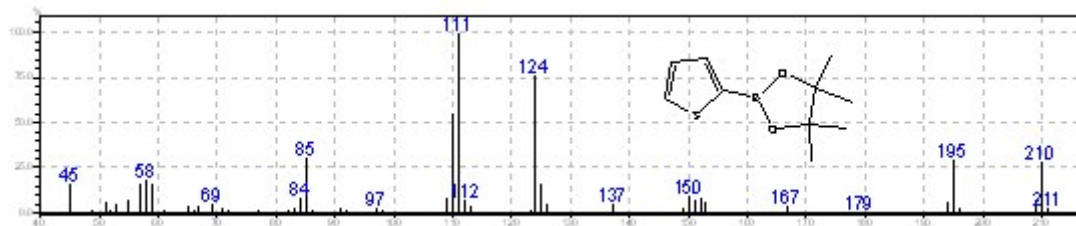
Figure S32. GC-MS of 5-bromo-acenaphthene



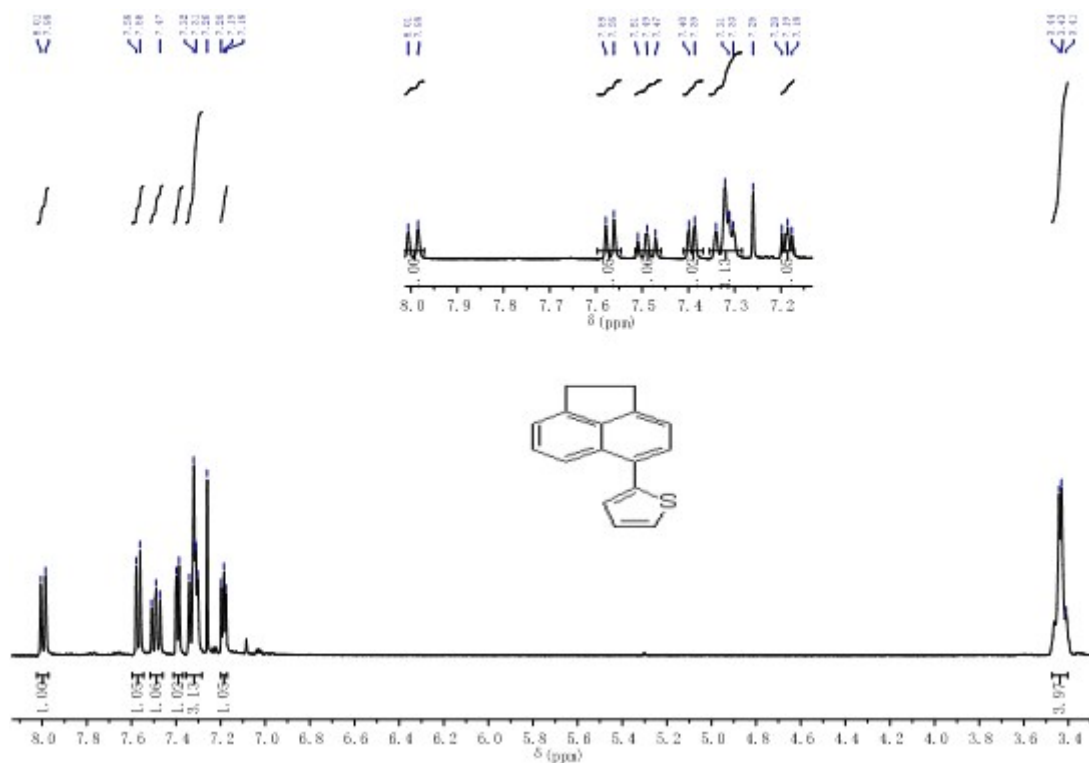
**Figure S33.**  $^1\text{H NMR}$  spectrum of 4, 4, 5, 5-tetramethyl-2-thiophen-2-yl-[1, 3, 2]dioxaborolane



**Figure S34.**  $^{13}\text{C NMR}$  spectrum of 4, 4, 5, 5-tetramethyl-2-thiophen-2-yl-[1, 3, 2]dioxaborolane



**Figure S35.** GC-MS of 4,4,5,5-tetramethyl-2-thiophen-2-yl-[1,3,2]dioxaborolane



**Figure S36.**  $^1\text{H}$  NMR spectrum of 2-acenaphthen-5-yl-thiophene



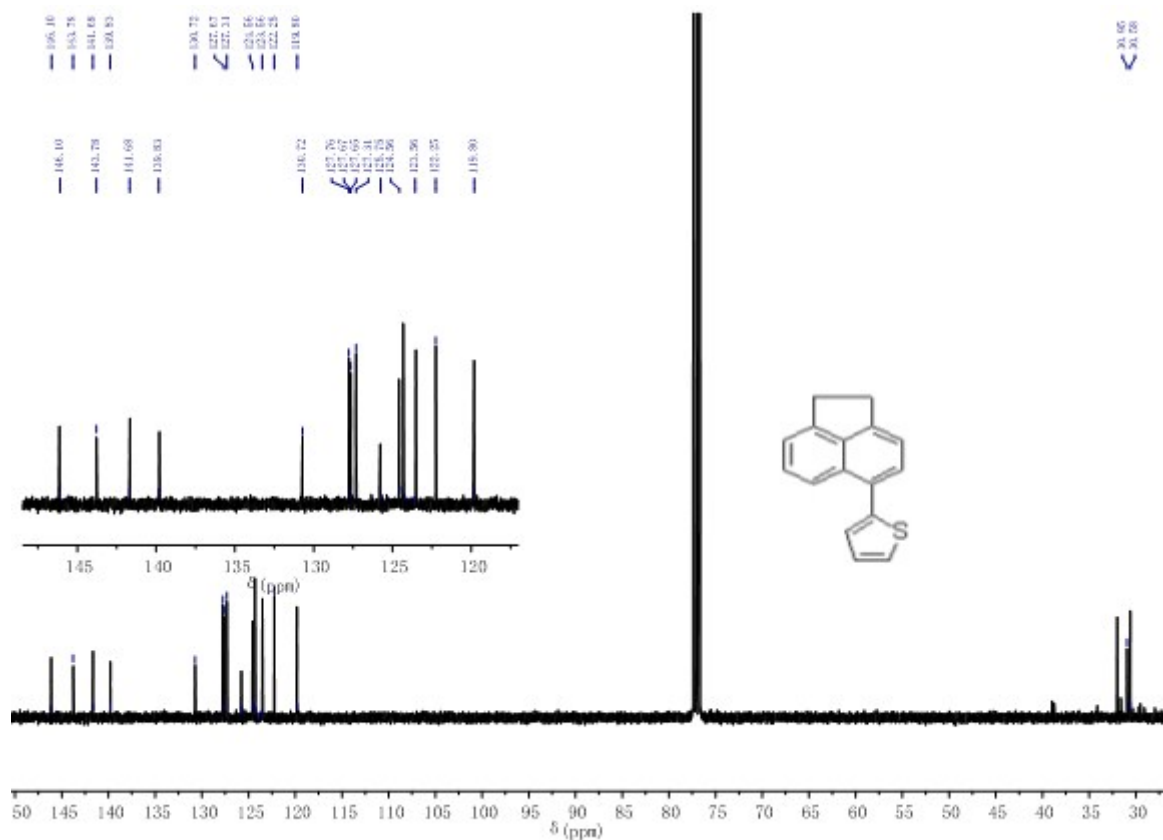


Figure S37.  $^{13}\text{C}$  NMR spectrum of 2-acenaphthen-5-yl-thiophene

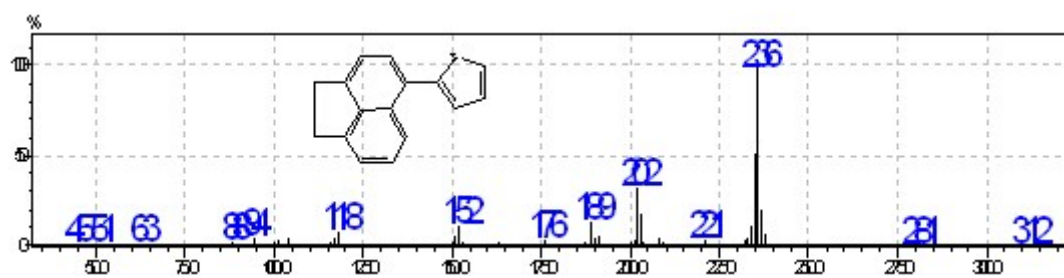


Figure S38. GC-MS of 2-acenaphthen-5-yl-thiophene

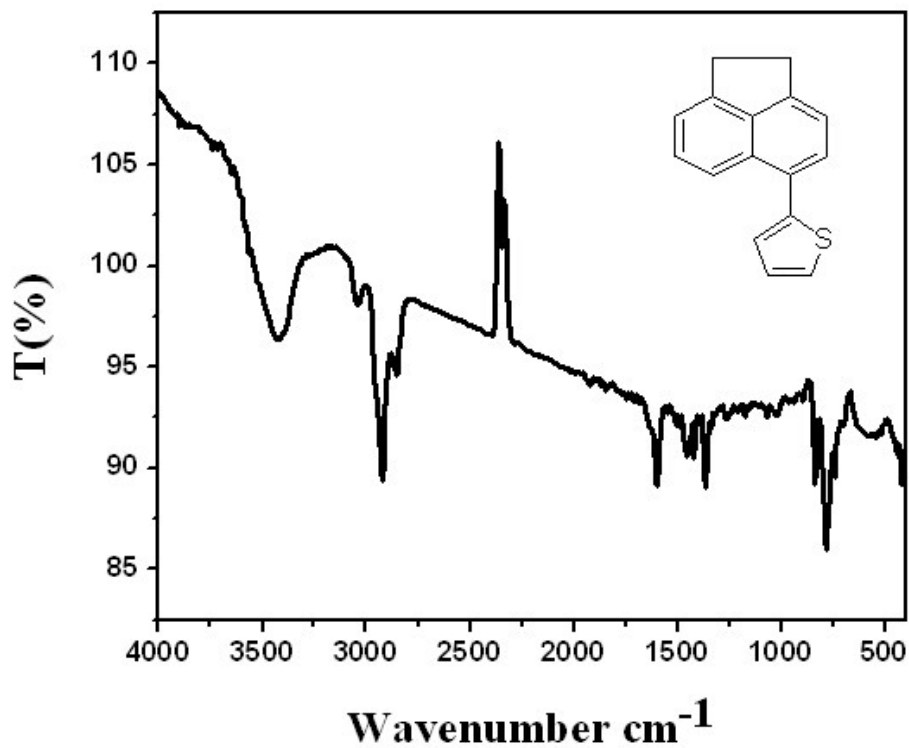


Figure S39. IR spectrum of 2-acenaphthen-5-yl-thiophene

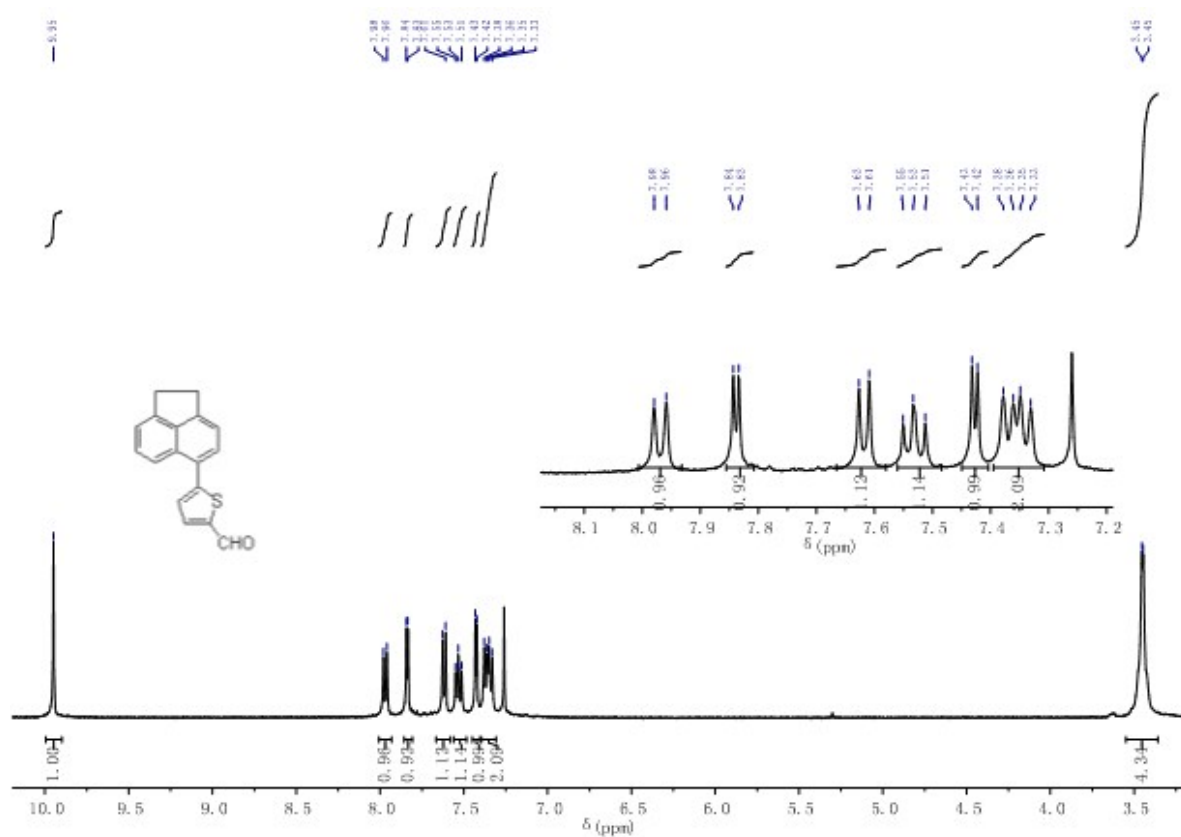
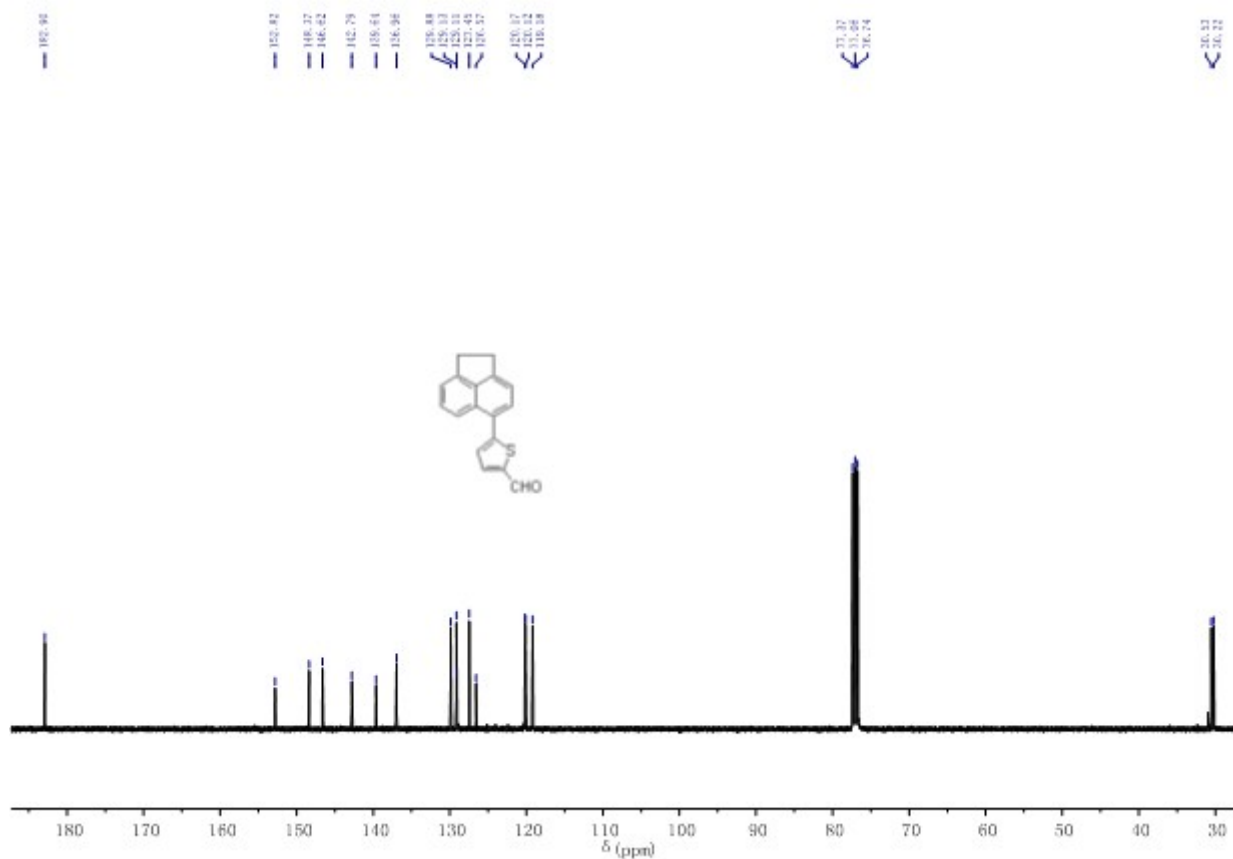
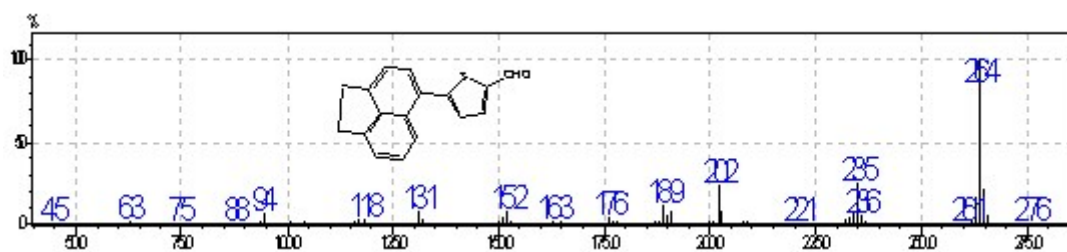


Figure S40. <sup>1</sup>H NMR spectrum of 5-acenaphthen-5-yl-thiophene-2-carbaldehyde



**Figure S41.**  $^{13}\text{C}$  NMR spectrum of 5-acenaphthen-5-yl-thiophene-2-carbaldehyde



**Figure S42.** GC-MS of 5-acenaphthen-5-yl-thiophene-2-carbaldehyde

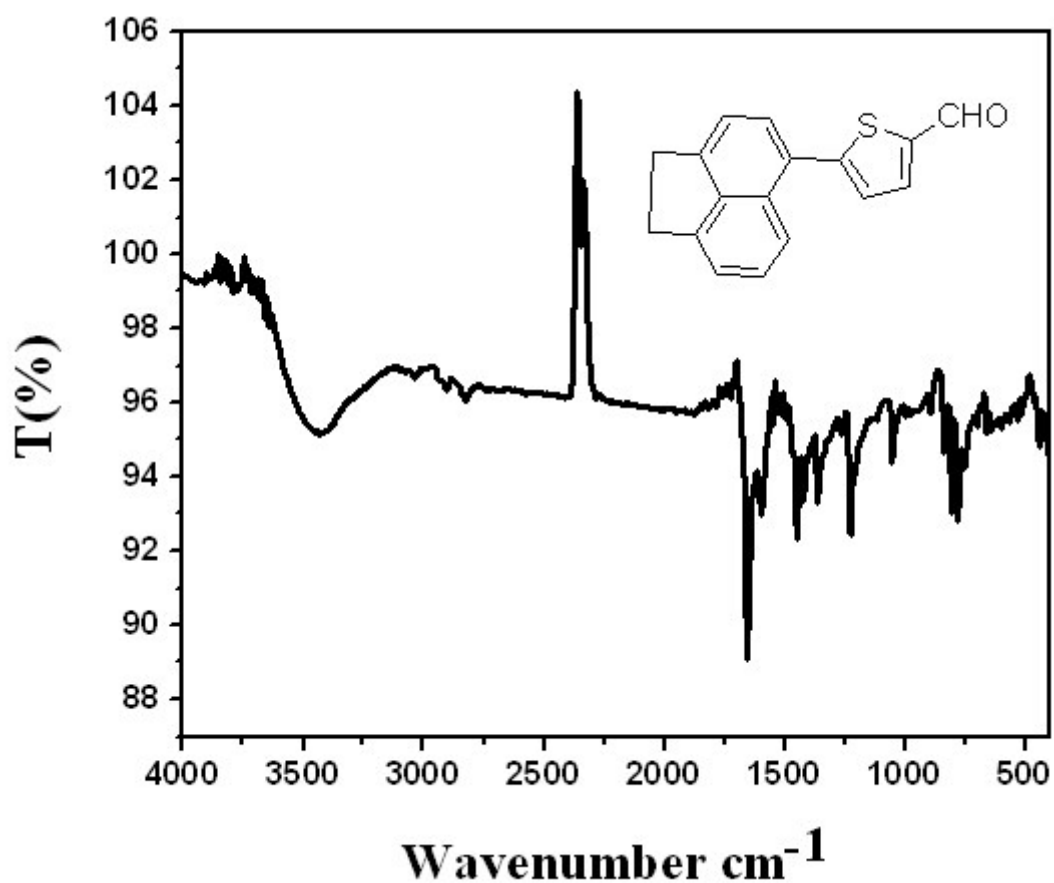


Figure S43. IR spectrum of 5-acenaphthen-5-yl-thiophene-2-carbaldehyde

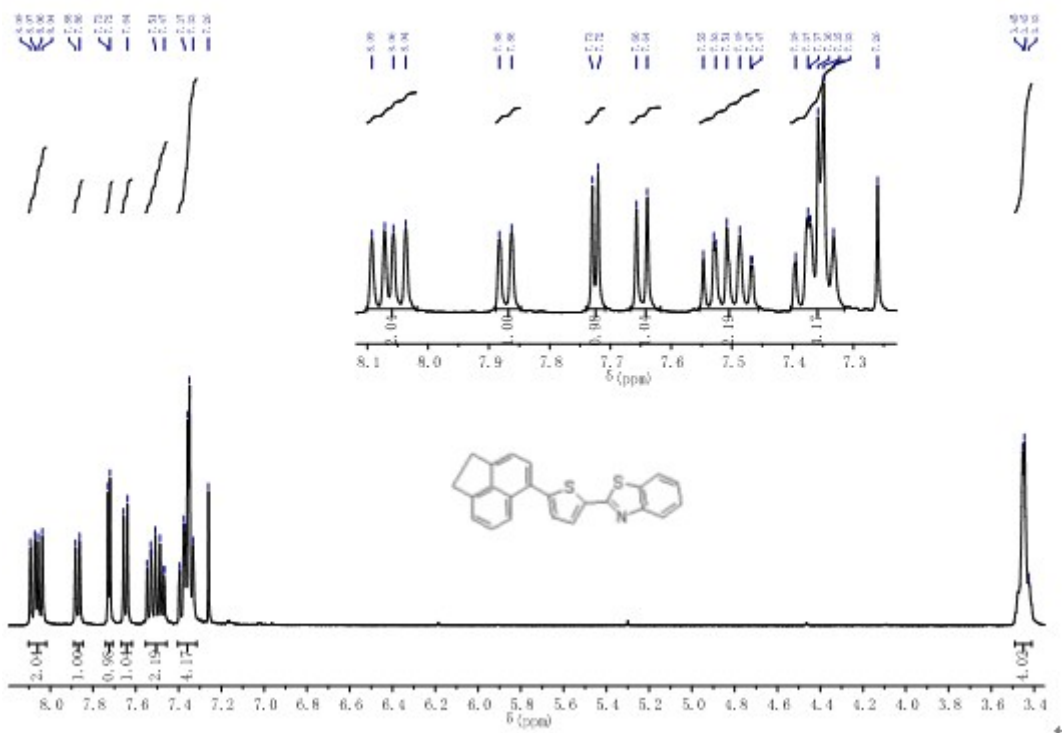


Figure S44. <sup>1</sup>H NMR spectrum of DTBT

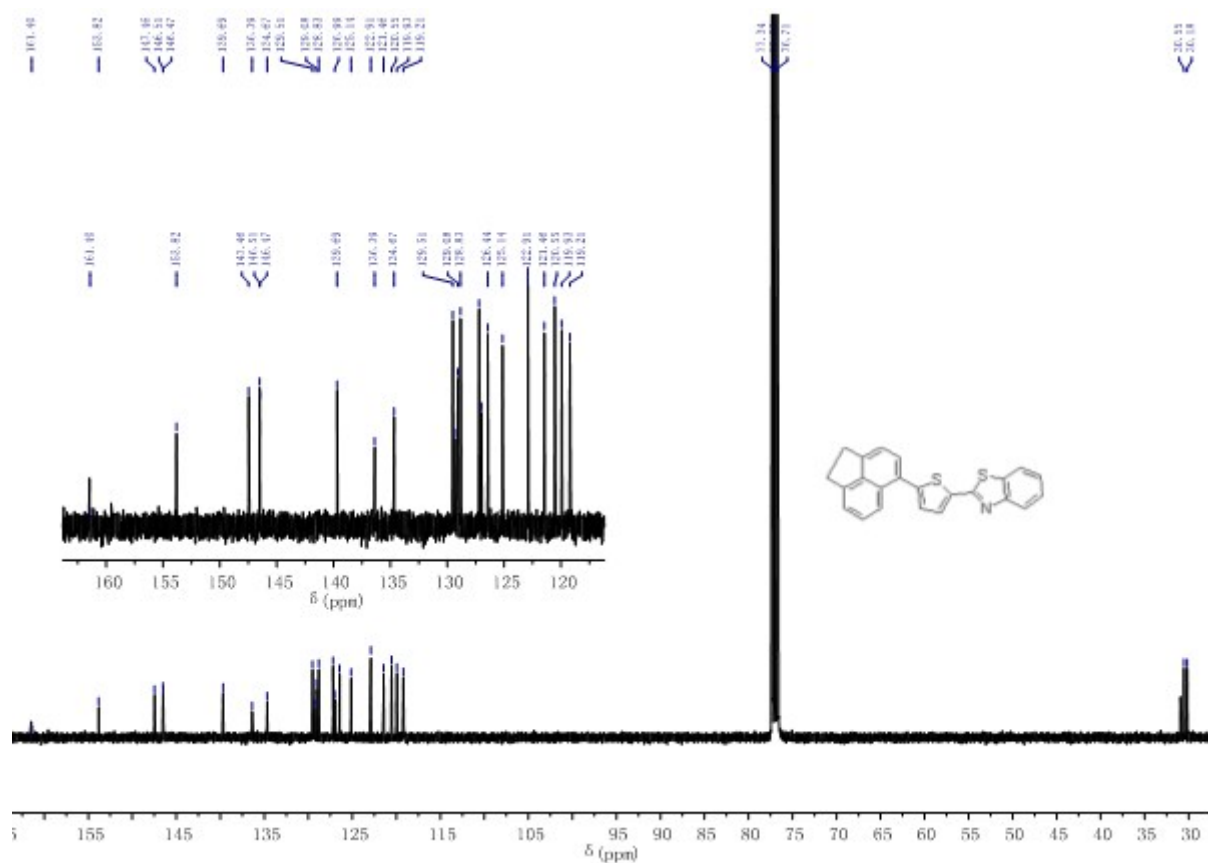


Figure S45.  $^{13}\text{C}$  NMR spectrum of DTBT

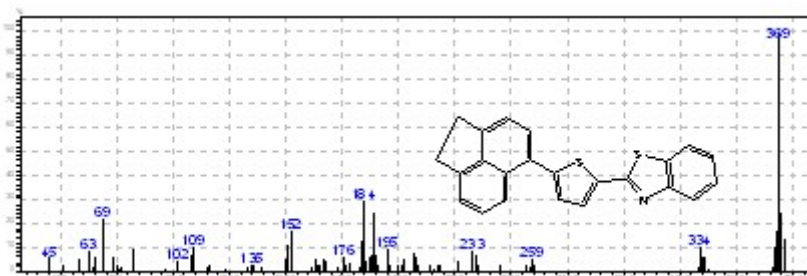
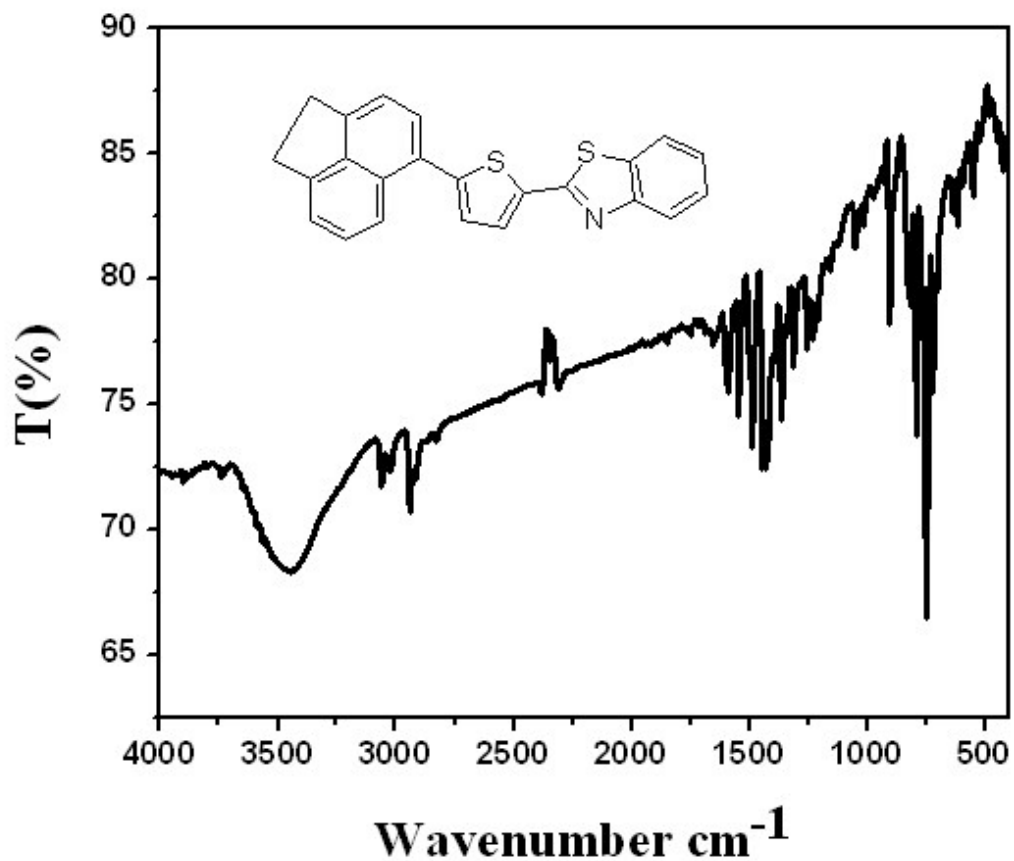
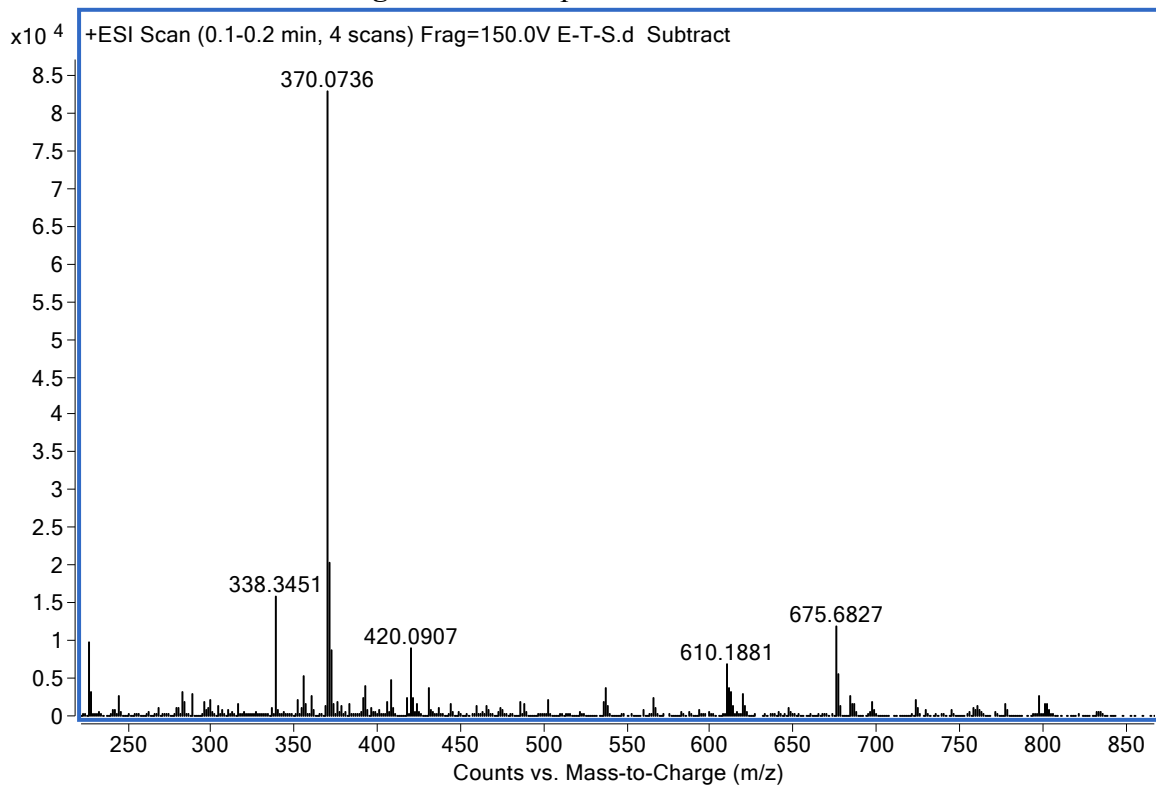


Figure S46. GC-MS of DTBT



**Figure S47. IR spectrum of DTBT**



**Figure S48. GC-MS of DTBT**

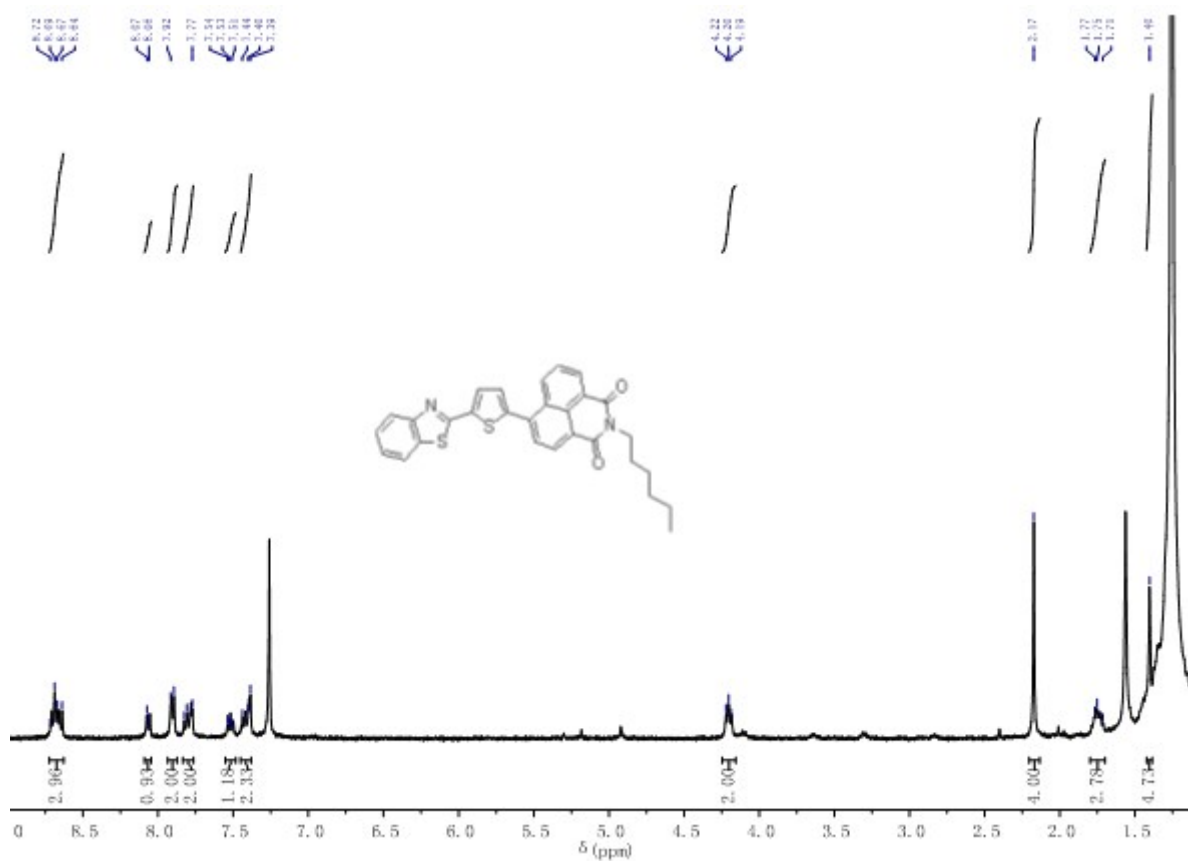


Figure S49. <sup>1</sup>H NMR spectrum of NTBT

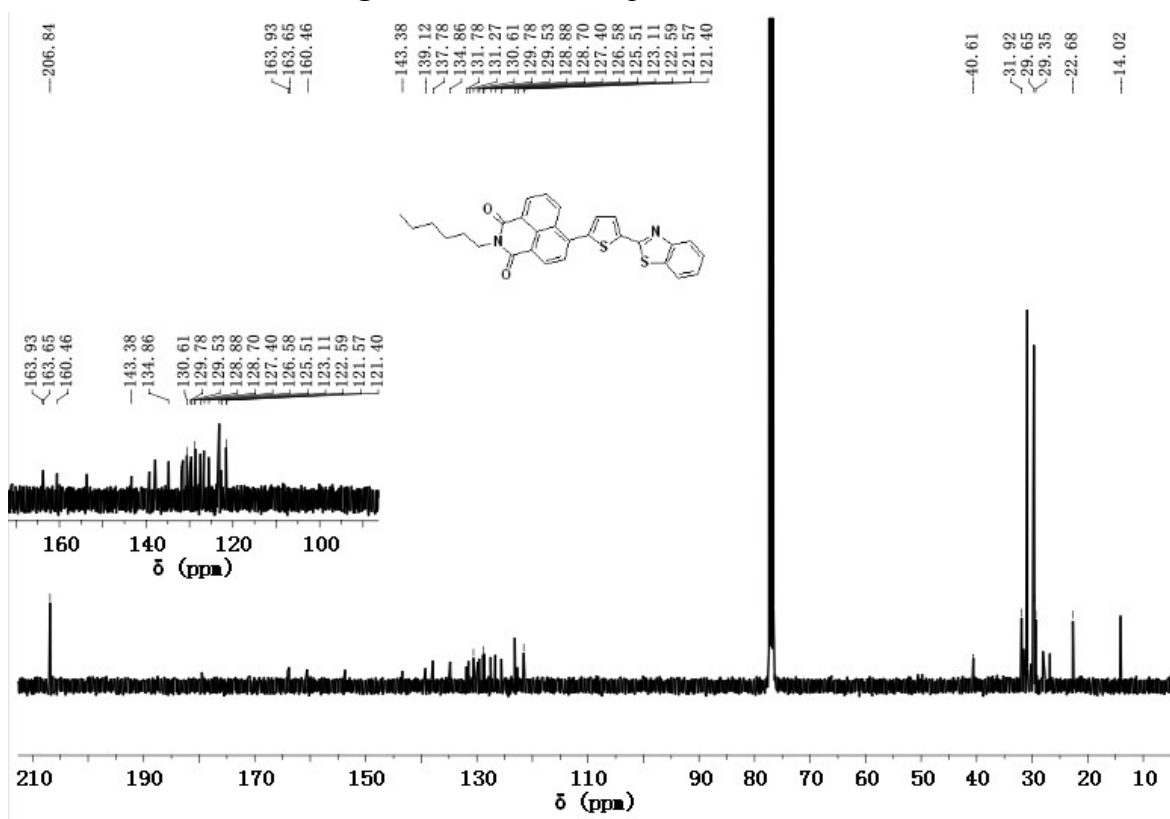
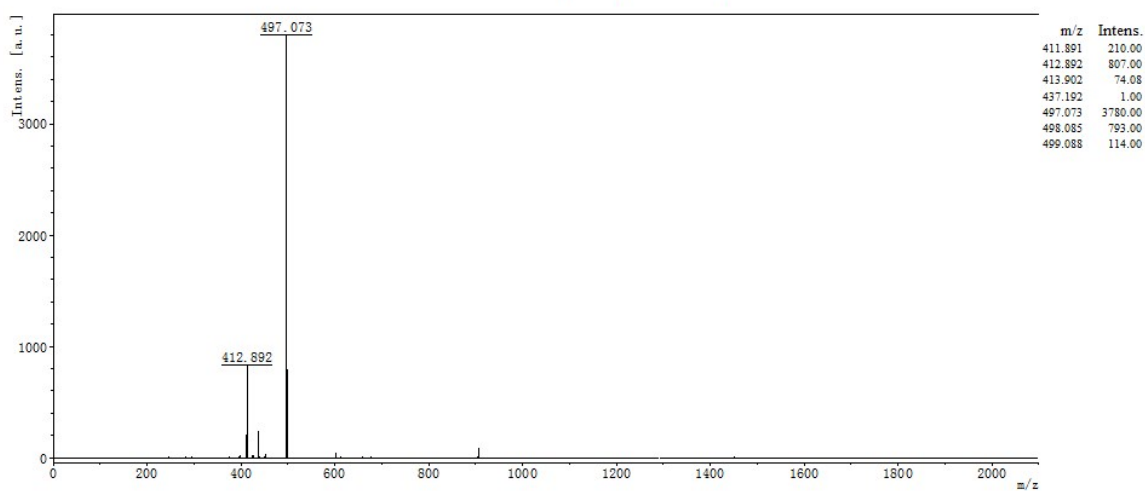


Figure S50. <sup>13</sup>C NMR spectrum of NTBT

Multiple Spectra Report



Acquisition Parameter

Figure S51. MALDI-TOF mass spectrum of NTBT

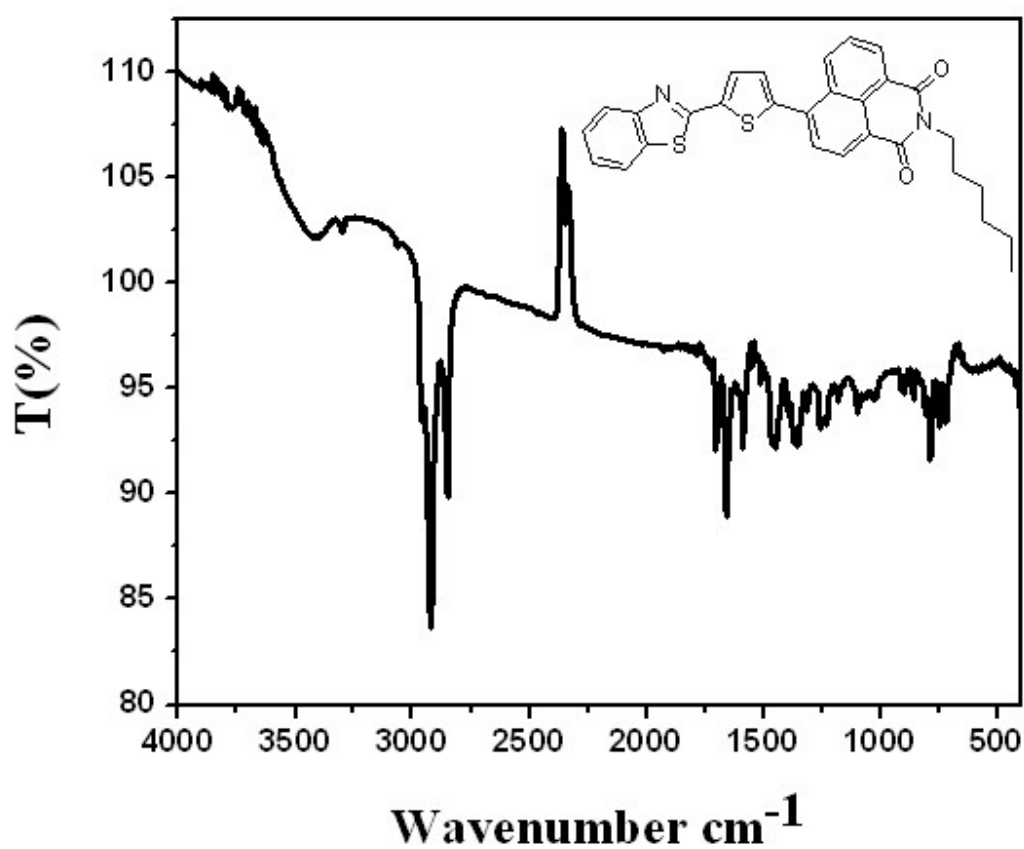


Figure S52. IR spectrum of NTBT